Tables of Molecular Vibrational Frequencies

Consolidated Volume II

T. Shimanouchi*

Department of Chemistry, University of Tokyo, Tokyo, Japan

The compilations of fundamental vibrational frequencies of molecules previously published as Tables of Molecular Vibrational Frequencies Part 5, Part 6, Part 7, and Part 8, which appeared in the Journal of Physical and Chemical Reference Data in 1972, 1973, and 1974, have been revised. This Consolidated Volume II includes data on a total of 212 molecules in addition to those on 223 molecules included in Volume I (NSRDS-NBS 39). Selected values of the fundamental vibrational frequencies are given for each molecule, together with observed infrared and Raman spectral data and citations to the original literature. The selection of vibrational fundamentals has been based on careful studies of the spectral data and comprehensive normal-coordinate analyses. An estimate of the accuracy of the selected values is included. The tables provide a convenient source of information for those who require vibrational energy levels and related properties in molecular spectroscopy, thermodynamics, analytical chemistry, and other fields of physics and chemistry.

Key words. Fundamental frequencies; infrared spectra; polyatomic molecules; Raman spectra; vibrational frequencies.

1. Introduction

Establishing the assignment of molecular vibrational frequencies has fundamental importance in elucidating various problems in physics and chemistry. The information concerning the force field and motion of atoms in a molecule can be most directly derived from its vibrational frequencies. If all the vibrational frequencies of a molecule are known, as well as the molecular structure, thermodynamic quantities can be easily computed on the ideal gas model. Thus, the need for a tabulation of evaluated reference data on molecular vibrational frequencies has often been felt by many investigators. In 1964 a project for producing such tables was initiated at the University of Tokyo in cooperation with the National Standard Reference Data System of the National Bureau of Standards. The evaluated data resulting from this project were first published in the three parts of Tables of Molecular Vibrational Frequencies [1] [1]. A Consolidated Volume [2] of these tables appeared in 1972 which includes revised versions of all the tables in [1] plus tables for 52 additional molecules (a total of 223 molecules). Tables covering 160 more molecules have appeared as Parts 5, 6, 7, and 8 of the series in earlier issues [3, 4,5,6] of this journal.

The present volume consists of Parts 5, 6, 7, and 8 after extensive revision in the light of new experimental data.

2. Molecules Selected and Their Ordering

The present volume contains tables of fundamental vibrational frequencies for 212 molecules. The molecules were selected from basic organic and inorganic molecules for which the vibrational assignments have been established with little ambiguity. The effort of extending the tables to many other important molecules is continuing in this laboratory. Diatomic molecules and electronically excited species are not included in this volume, since [7, 8, 9] contain good compilations of data for them. Rotational isomers are treated as independent molecular species, and a separate table is made for each of the isomers. When the gas and liquid state spectra are significantly different from each other, they are tabulated separately.

The molecules are ordered according to the following rules:

(a) Number of carbon atoms.

(b) Total number of atoms.

(c) Molecular shape: linear, planar, and non-planar.

(d) Molecular symmetry, in descending order of the number of symmetry elements. Isotopically substituted molecules directly follow the normal species regardless of their symmetry.

(e) Atomic number of main atoms.

(f) Atomic number of the other atoms.

Molecules are first divided into groups by the items (a) and (b) and the ordering of molecules in each group is given by the items (c), (d), (e), and (f). A complete list in the order presented is given at the beginning of the tables. Indices by compound name and empirical formula follow the tables.

3. Description of the Tables

3.1. Symmetry

The symmetry (point group) of each molecule is given by the Schoenflies notation. Detailed discussions of symmetry properties will be found in [10] and [11].

3.2. Symmetry Number

The symmetry number, σ, is used in the calculation of thermodynamic quantities. It is the number of indistinguishable positions into which the molecule can be transformed by simple rigid rotations. A general discussion and pertinent formulas may be found in [11], page 508.

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[1] Figures in brackets indicate the literature references in section 5.

*Present address: College of Information Sciences, Third Cluster of Colleges, The University of Tsukuba, Sakura, Ibaraki 300-31, Japan.

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3.3. Symmetry Species

In the table the normal modes are divided into the symmetry species of the point group to which the molecule belongs. The ordering of species in each point group is given in table I, which is a summary of tables 12–30 of [11]. When a molecule has two or three planes of symmetry, the relationship between the vibrational modes and symmetry species cannot be defined uniquely. In such cases we generally follow the notation adopted in [11].

TABLE I. Ordering of symmetry species

(In the present article small letters are used to designate the species of fundamental frequencies)

Point group	Symmetry species
C_2	A, B
C_s	A′, A″
C_i	A_g, A_u
C_{2v}	A_1, A_2, B_1, B_2
C_{2h}	A_g, A_u, B_g, B_u
D_2	A, B_1, B_2, B_3
D_{2h}	A_g, A_u, B_{1g}, B_{1u}, B_{2g}, B_{2u}, B_{3g}, B_{3u}
C_{3v}	A_1, A_2, E
D_3	A_1, A_2, E
C_{5v}	A_1, A_2, E_1, E_2
$C_{\infty v}$	Σ^+, Σ^-, π, Δ, Φ, ...
C_{4v}, D_4, D_{2d}	A_1, A_2, B_1, B_2, E
C_{6v}, D_6	A_1, A_2, B_1, B_2, E_1, E_2
D_{3d}	A_{1g}, A_{1u}, A_{2g}, A_{2u}, E_g, E_u
D_{4d}	A_1, A_2, B_1, B_2, E_1, E_2, E_3
D_{3h}	A_1', A_1'', A_2', A_2'', E′, E″
D_{5h}	A_1', A_1'', A_2', A_2'', E_1', E_1'', E_2', E_2''
D_{4h}	A_{1g}, A_{1u}, A_{2g}, A_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{2u}, E_g, E_u
D_{6h}	A_{1g}, A_{1u}, A_{2g}, A_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{2u}, E_{1g}, E_{1u}, E_{2g}, E_{2u}
$D_{\infty h}$	Σ_g^+, Σ_u^+, Σ_g^-, Σ_u^-, π_g, π_u, Δ_g, Δ_u, Φ_g, Φ_u, ...
C_3	A, E
C_6	A, B, E_1, E_2
S_6	A_g, A_u, E_g, E_u
C_{3h}	A′, A″, E′, E″
C_{4h}	A_g, A_u, B_g, B_u, E_g, E_u
C_{6h}	A_g, A_u, B_g, B_u, E_{1g}, E_{1u}, E_{2g}, E_{2u}
T_d, O	A_1, A_2, E, F_1, F_2
O_h	A_{1g}, A_{1u}, A_{2g}, A_{2u}, E_g, E_u, F_{1g}, F_{1u}, F_{2g}, F_{2u}
T	A, E, F

3.4. Numbering of Frequencies

The numbering is indicated by ν_i given in the second column of each table. The normal modes are first grouped into symmetry species, and then those in each species are ordered from higher to lower values of the frequency. However, we always denote the bending vibration of a linear triatomic molecule as ν_2, following the widely accepted nomenclature [12]. For the C_2X_6 type of molecule we adopt the numbering given in[11], although it is based on D_{3h} symmetry. For some deuterated compounds the frequencies are arranged so that the same ν_i numbering is given to the corresponding vibrational modes of deuterated and normal compounds.

3.5. Approximate Type of Mode

The approximate type of mode given in the third column of each table is the local symmetry coordinate which makes the maximum contribution to the normal mode. Local symmetry coordinates are defined for several chemical groups in table II. It should be emphasized that two or more local symmetry coordinates are often coupled strongly in a normal coordinate, and the approximate type of mode given in the table has only limited significance in such a case.

TABLE II. Definition of local symmetry coordinates

(a) Local symmetry coordinates for the CH_3 group (see fig. 1a)

CH_3 symmetrical stretching: $(\Delta r_1 + \Delta r_2 + \Delta r_3) / \sqrt{3}$

CH_3 degenerate stretching: $(2\Delta r_1 - \Delta r_2 - \Delta r_3) / \sqrt{6}$

$(\Delta r_2 - \Delta r_3) / \sqrt{2}$

CH_3 symmetrical deformation:

$(\Delta\alpha_{23} + \Delta\alpha_{31} + \Delta\alpha_{12} - \Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3) / \sqrt{6}$

CH_3 degenerate deformation: $(2\Delta\alpha_{23} - \Delta\alpha_{31} - \Delta\alpha_{12}) / \sqrt{6}$

$(\Delta\alpha_{31} - \Delta\alpha_{12}) / \sqrt{2}$

CH_3 rocking: $(2\Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3) / \sqrt{6}$

$(\Delta\beta_2 - \Delta\beta_3) / \sqrt{2}$

(b) Local symmetry coordinates for the CH_2 group (see fig. 1b)

CH_2 symmetrical stretching: $(\Delta r_1 + \Delta r_2) / \sqrt{2}$

antisymmetrical stretching: $(\Delta r_1 - \Delta r_2) / \sqrt{2}$

CH_2 scissors: $(4\Delta\alpha - \Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{2Y}) / \sqrt{20}$

CH_2 wagging: $(\Delta\beta_{1X} + \Delta\beta_{2X} - \Delta\beta_{1Y} - \Delta\beta_{2Y}) / 2$

CH_2 twisting: $(\Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} + \Delta\beta_{2Y}) / 2$

CH_2 rocking: $(\Delta\beta_{1X} - \Delta\beta_{2X} + \Delta\beta_{1Y} - \Delta\beta_{2Y}) / 2$.

(c) Local symmetry coordinates for the CH group (see fig. 1c)

CH stretching: Δr_{CH}

CH bending: $(2\Delta\beta_{HX} - \Delta\beta_{HY} - \Delta\beta_{HZ}) / \sqrt{6}$

$(\Delta\beta_{HY} - \Delta\beta_{HZ}) / \sqrt{2}$

(d) Local symmetry coordinates for the planar CH_2 group (see fig. 1d)

CH_2 symmetrical stretching: $(\Delta r_1 + \Delta r_2) / \sqrt{2}$

CH_2 antisymmetrical stretching: $(\Delta r_1 - \Delta r_2) / \sqrt{2}$

CH_2 scissors: $(2\Delta\alpha - \Delta\beta_1 - \Delta\beta_2) / \sqrt{6}$

CH_2 rocking: $(\Delta\beta_1 - \Delta\beta_2) / \sqrt{2}$

CH_2 wagging: $\Delta\theta \cdot \sin\alpha$.

(e) Local symmetry coordinates for the planar CH group (see fig. 1e)

CH stretching: Δr_{CH}

in-plane CH bending: $(\Delta\beta_{HX} - \Delta\beta_{HY}) / \sqrt{2}$

out-of-plane CH bending: $\Delta\theta_H \cdot \sin\gamma_{XY}$.

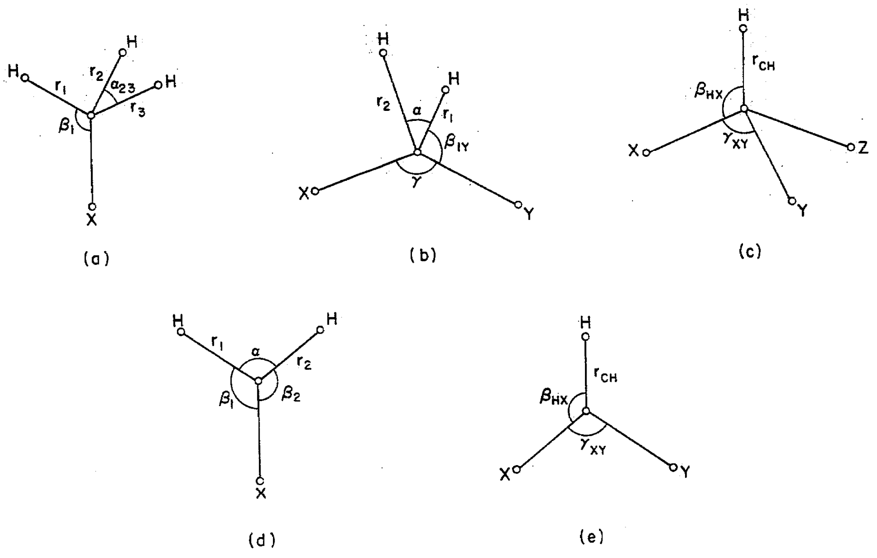

FIGURE 1. Parameters of methyl, methylene, and methine groups.

The following abbreviations are used for the type of mode:

stretch.	stretching
deform.	deformation
rock.	rocking
twist.	twisting
wag.	wagging
scis.	scissors
bend.	bending
sym. or s-	symmetrical
anti. or a-	antisymmetrical
deg. or d-	degenerate
ip-	in-plane
op-	out-of-plane

The plane to which the in-plane and out-of-plane expressions refer is the molecular plane of a planar molecule or the symmetry plane of a general molecule belonging to point group C_s. Local symmetry coordinates of the CX_3 groups attached to a relatively large molecule are designated as s-stretch, s-deform., d-stretch., and d-deform. In such a molecule with low symmetry none of the normal vibrations are genuinely "symmetrical" or "degenerate" with respect to the three-fold symmetry axis of the CX_3 group. However, the notation is retained because it is convenient for indicating the correspondence between similar modes in large and small molecules.

3.6. Selected Value of Frequency [2]

The fundamental frequency ν_i is defined as the difference between the term values $G(v_i = 1$, all other $v_j = 0)$ and $G(v_i = 0$, and other $v_j = 0)$ expressed in cm^{-1}. Fundamental frequencies rather than harmonic frequencies (ω_j) are listed in the table. Although harmonic frequencies are of greater physical significance, they are accurately known only for a small number of polyatomic molecules. The selected values are rounded to the nearest 1 cm^{-1}.

The letter code, A, B, C, D, or E following the selected value of frequency indicates the evaluator's judgment of the accuracy of the value. The basis for estimating accuracy of an observed frequency is given in table III, together with the range of uncertainty in cm^{-1} for each grade.

[2] In keeping with the universally accepted convention in molecular spectroscopy, the fundamental frequencies are expressed in their wavenumber (cm^{-1}) equivalents. The actual frequency in units of hertz may be obtained by multiplying the numbers in these tables by the speed of light expressed in centimeters per second.

TABLE III. Uncertainty code for the selected values of frequencies

Notation	Uncertainty	Basis [a]
	cm^{-1}	
A	0 ~ 1	(i) Gas, grating spectrometer, rotational fine structure accurately analyzed. (ii) Gas, grating spectrometer, a sharp Q branch.
B	1 ~ 3	(i) Gas, grating spectrometer, rotational fine structure partly analyzed. (ii) Gas, prism spectrometer, fairly high resolution (e.g., 700 ~ 1000 cm^{-1} for NaCl prism).
C	3 ~ 6	(i) Gas, prism spectrometer, low resolution (e.g., 1000 ~ 2000 cm^{-1} for NaCl prism). (ii) Solid, liquid or solution, accurate measurement.
D	6 ~ 15	(i) Gas, prism spectrometer, very low resolution (e.g., > 2000 cm^{-1} for NaCl prism). (ii) Solid, liquid or solution, inaccurate measurement.
E	15 ~ 30	(i) Value estimated from Fermi resonance doublet. (ii) Value estimated from overtone or combination tone. (iii) Calculated frequency.

[a] The uncertainty assigned here to each method of measurement is a typical value; greater accuracy is often achieved with some of the methods.

Frequencies derived from infrared and Raman measurements in the gaseous state are chosen unless otherwise mentioned. When a detailed analysis of the rotational fine structure of an infrared band is available, the band center ν_0 is chosen as the fundamental frequency and given the uncertainty code A (see below). For a well-analyzed perpendicular band of a symmetric top molecule, the frequency listed contains the nonvibrational part $A' \zeta^2$, where A' is the rotational constant of the vibrational level and ζ is the Coriolis coupling constant. This is in accord with the definition of ν_0 given in [11], page 404 and equation (IV, 60).

When the spectra in the gaseous state are not available, the frequencies observed in the liquid or solid state are listed. When no spectral data have been obtained, the results of normal vibration calculations or of some other methods of estimating frequencies are listed with the grade D or E.

The torsional frequency may be calculated using the barrier height and reduced moment derived from microwave spectroscopy. The value obtained in this way is given as MW (frequency in cm^{-1}) in the "Comments" column or as a footnote for comparison with the value observed or calculated by the normal coordinate treatment. Microwave data are taken from [13] unless otherwise noted.

For many molecules the assignments given in the literature have been checked by normal vibration calculations carried out in this laboratory as part of the project. Revisions in some assignments have been made as a result of these calculations. The details of the normal coordinate treatment and evaluation of force constants may be found in [14].

Thermodynamic quantities may be computed in most cases by employing the harmonic oscillator partition function and by assuming that the harmonic frequencies are not much different from the fundmental frequencies given here. Such an approximation is not adequate, however, for molecules with highly anharmonic motions such as internal rotation, inversion, and ring-puckering. The vibrational partition function should be formed for these molecules by summing the terms due to the individual energy levels.

3.7. Infrared and Raman Spectra

The observed infrared and Raman frequencies are given in the fifth and sixth columns of each table. Rough estimates of relative intensities, band shapes, and polarization characteristics are also given. An additional significant figure is included here when warranted. The abbreviations used here are as follows:

VS	very strong
S	strong
M	medium
W	weak
VW	very weak
ia	inactive
b	broad
vb	very broad
sh	shoulder
p	polarized
dp	depolarized

For some molecules the relative intensities of Raman lines are indicated by the numbers from one to ten in accordance with the tradition widely used. These estimates of intensity are taken from the original references without any attempt at critical evaluation.

3.8. Comments

In the last column of each table brief comments are added to give special information which is not indicated in the preceding columns. The abbreviations used in this column are as follows:

FR Fermi resonance with an overtone or a combination tone indicated in the parentheses.

OC Frequency estimated from an overtone or a combination tone indicated in the parentheses.

CF Calculated frequency.

SF Calculation shows that frequency approximately equals that of the vibration indicated in the parentheses.

OV Overlapped by the band indicated in the parentheses.

MW Torsional frequency calculated from microwave spectroscopic data.

RP Frequency determined by the Ritz principle.

EL Derived from analysis of electronic transitions.

3.9. Footnotes and References

The footnote is used to supply other necessary information which cannot be placed simply in the column of Comments. The references accompanying the table are not comprehensive. Only the papers relevant to the present tabulation are cited. The abbreviations IR, R, MW, and Th stand for infrared, Raman, microwave, and theoretical, respectively.

4. Acknowledgments

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List of Tables of Molecular Vibrational Frequencies

C_0–triatomic molecules

No. 1 Krypton difluoride KrF_2
No. 2 Nitrogen dioxide $^{14}NO_2$
No. 3 Nitrogen dioxide $^{15}NO_2$
No. 4 Ozone $^{16}O_3$
No. 5 Ozone $^{18}O_3$
No. 6 Water $H_2{}^{18}O$
No. 7 Sulfur dioxide $S^{18}O_2$
No. 8 Sulfur dichloride SCl_2
No. 9 Germanium (II) chloride $GeCl_2$
No. 10 Tin (II) fluoride SnF_2
No. 11 Tin (II) chloride $SnCl_2$
No. 12 Tin (II) bromide $SnBr_2$
No. 13 Lead (II) fluoride PbF_2
No. 14 Lead (II) chloride $PbCl_2$
No. 15 Nitrosyl fluoride $^{16}O^{14}NF$
No. 16 Nitrosyl fluoride $^{16}O^{15}NF$
No. 17 Nitrosyl fluoride $^{18}O^{14}NF$
No. 18 Nitrosyl fluoride $^{18}O^{15}NF$
No. 19 Nitrosyl chloride $^{16}O^{14}NCl$
No. 20 Nitrosyl chloride $^{16}O^{15}NCl$
No. 21 Nitrosyl chloride $^{18}O^{14}NCl$
No. 22 Nitrosyl chloride $^{18}O^{15}NCl$
No. 23 Nitrosyl bromide $^{16}O^{14}NBr$
No. 24 Nitrosyl bromide $^{16}O^{15}NBr$
No. 25 Nitrosyl bromide $^{18}O^{15}NBr$
No. 26 Hypofluorous acid HOF
No. 27 Hypochlorous acid HOCl
No. 28 Hypochlorous acid–d DOCl
No. 29 Thionitrosyl–S–fluoride NSF
No. 30 Thionitrosyl–S–chloride NSCl

C_0–four–atomic molecules

No. 31 Boron trifluoride $^{10}BF_3$
No. 32 Boron trifluoride $^{11}BF_3$
No. 33 Sulfur trioxide SO_3
No. 34 Ammonia–t_3 NT_3
No. 35 Nitrogen trifluoride $^{15}NF_3$
No. 36 Aluminum trichloride $AlCl_3$
No. 37 Phosphorus triiodide PI_3
No. 38 Arsenic trifluoride AsF_3
No. 39 Arsenic triiodide AsI_3
No. 40 trans–1,2–Difluorodiazine N_2F_2
No. 41 Nitryl fluoride $F^{14}NO_2$
No. 42 Nitryl fluoride $F^{15}NO_2$
No. 43 Nitryl chloride $Cl^{14}NO_2$
No. 44 Nitryl chloride $Cl^{15}NO_2$

No. 45 Chlorine trifluoride ClF_3
No. 46 Bromine trifluoride BrF_3
No. 47 Hydrogen peroxide H_2O_2
No. 48 Hydrogen persulfide H_2S_2
No. 49 Difluoro disulphane F_2S_2
No. 50 Hydrazoic acid HN_3
No. 51 Hydrazoic acid DN_3
No. 52 Difluoroamine NF_2H
No. 53 Chlorodifluoroammonia $NClF_2$
No. 54 Dichlorofluoroammonia NCl_2F
No. 55 Thionyl fluoride SOF_2
No. 56 Thionyl chloride $SOCl_2$
No. 57 Thionyl bromide $SOBr_2$

C_0–five–atomic molecules

No. 58 Titanium tetrachloride $TiCl_4$
No. 59 Titanium tetrabromide $TiBr_4$
No. 60 Titanium tetraiodide TiI_4
No. 61 Zirconium tetrachloride $ZrCl_4$
No. 62 Zirconium tetrabromide $ZrBr_4$
No. 63 Zirconium tetraiodide ZrI_4
No. 64 Ruthenium tetroxide RuO_4
No. 65 Hafnium tetrachloride $HfCl_4$
No. 66 Hafnium tetrabromide $HfBr_4$
No. 67 Hafnium tetraiodide HfI_4
No. 68 Osmium tetroxide $Os^{16}O_4$
No. 69 Osmium tetroxide $Os^{18}O_4$
No. 70 Thionitrosyl trifluoride NSF_3
No. 71 Trifluorosilane $SiHF_3$
No. 72 Trifluorosilane–d $SiDF_3$
No. 73 Trichlorosilane $SiHCl_3$
No. 74 Trichlorosilane–d $SiDCl_3$
No. 75 Tribromosilane $SiHBr_3$
No. 76 Phosphoryl fluoride POF_3
No. 77 Phosphoryl chloride $POCl_3$
No. 78 Phosphoryl bromide $POBr_3$
No. 79 Thiophosphoryl trifluoride PSF_3
No. 80 Thiophosphoryl trichloride $PSCl_3$
No. 81 Perchlorylfluoride $^{35}ClO_3F$
No. 82 Vanadyl(V) chloride $VOCl_3$
No. 83 Permanganyl fluoride MnO_3F
No. 84 Germyl fluoride GeH_3F
No. 85 Germyl fluoride–d_3 GeD_3F
No. 86 Germyl chloride GeH_3Cl
No. 87 Germyl chloride–d_3 GeD_3Cl
No. 88 Germyl bromide GeH_3Br
No. 89 Germyl bromide–d_3 GeD_3Br
No. 90 Germyl iodide GeH_3I
No. 91 Germyl iodide–d_3 GeD_3I
No. 92 Trichlorogermane $GeHCl_3$
No. 93 Tribromogermane $GeHBr_3$
No. 94 Rhenium (VII) oxide chloride ReO_3Cl
No. 95 Rhenium (VII) oxide bromide ReO_3Br
No. 96 Sulfuryl fluoride SO_2F_2
No. 97 Sulfuryl chloride SO_2Cl_2
No. 98 Dichlorosilane SiH_2Cl_2
No. 99 Dichlorosilane–d_2 SiD_2Cl_2
No. 100 Dibromosilane SiH_2Br_2
No. 101 Selenium dioxide difluoride SeO_2F_2
No. 102 Nitric acid $H^{14}NO_3$
No. 103 Nitric acid–d $D^{14}NO_3$
No. 104 Nitric acid $H^{15}NO_3$
No. 105 Nitric acid–d $D^{15}NO_3$
No. 106 Fluoronitrate $FO^{14}NO_2$
No. 107 Fluoronitrate $FO^{15}NO_2$
No. 108 Chloronitrate $ClO^{14}NO_2$
No. 109 Chloronitrate $ClO^{15}NO_2$
No. 110 Phosphoryl dichlorofluoride $POCl_2F$
No. 111 Phosphoryl dibromofluoride $POBr_2F$
No. 112 Thiophosphoryl chlorodifluoride $PSClF_2$
No. 113 Thiophosphoryl dichlorofluoride $PSCl_2F$

C_0–six–atomic molecules

No. 114 Phosphorus pentafluoride PF_5
No. 115 Phosphorus trichloride difluoride PCl_3F_2
No. 116 Phosphorus pentachloride PCl_5
No. 117 Vanadium pentafluoride VF_5
No. 118 Arsenic pentafluoride AsF_5
No. 119 Antimony pentachloride $SbCl_5$

C_0–seven–atomic molecules

No. 120 Tellurium hexafluoride TeF_6
No. 121 Iridium(VI)fluoride IrF_6
No. 122 Sulfur chloride pentafluoride $SClF_5$
No. 123 Tungsten chloride pentafluoride $WClF_5$

C_0–eight–atomic molecules

No. 124 Iodine heptafluoride IF_7
No. 125 Digermane GeH_3GeH_3
No. 126 Digermane–d_6 GeD_3GeD_3

C_1–triatomic molecules

No. 127 Cyanogen fluoride FCN
No. 128 Cyanogen iodide ICN

C_1–four–atomic molecules

No. 129 Carbonyl fluoride COF_2
No. 130 Carbonyl chloride $COCl_2$
No. 131 Carbonyl bromide $COBr_2$
No. 132 Thiocarbonyl fluoride SCF_2
No. 133 Thiocarbonyl chloride $CSCl_2$
No. 134 Isocyanic acid HNCO
No. 135 Isocyanic acid–d DNCO
No. 136 Carbonyl chlorofluoride COClF
No. 137 Carbonyl bromochloride COBrCl
No. 138 Thiocarbonyl bromochloride CSBrCl

C_1–five–atomic molecules

No. 139 Trifluoromethane–d CDF_3
No. 140 Chlorotrifluoromethane $CClF_3$
No. 141 Bromotrifluoromethane $CBrF_3$
No. 142 Trifluoroiodomethane CF_3I
No. 143 Trichlorofluoromethane CCl_3F
No. 144 Trichloroiodomethane CCl_3I
No. 145 Tribromofluoromethane CBr_3F
No. 146 Dichlorodifluoromethane CCl_2F_2
No. 147 Dibromodifluoromethane CBr_2F_2
No. 148 Bromodichlorofluoromethane $CBrCl_2F$
No. 149 Dibromochlorofluoromethane CBr_2ClF

C_1–six–atomic molecules

No. 150 Borine Carbonyl $^{10}BH_3CO$
No. 151 Borine Carbonyl–d_3 $^{10}BD_3CO$
No. 152 Borine Carbonyl $^{11}BH_3CO$
No. 153 Borine Carbonyl–d_3 $^{11}BD_3CO$
No. 154 Methylmercuric iodide CH_3HgI

C_1–eight–atomic molecules

No. 155 Methylsilane CH_3SiH_3
No. 156 Methylsilane–d_3 CH_3SiD_3
No. 157 Methylgermane CH_3GeH_3
No. 158 Methyl–d_3–germane CD_3GeH_3
No. 159 Methyltriiodogermane CH_3GeI_3
No. 160 Methylstannane CH_3SnH_3
No. 161 Methylstannane–d_3 CH_3SnD_3
No. 162 Methyl–d_3–stannane CD_3SnH_3

C_2–four–atomic molecules

No. 163 Cyanogen C_2N_2
No. 164 Dichloroacetylene C_2Cl_2
No. 165 Dibromoacetylene C_2Br_2
No. 166 Diiodoacetylene C_2I_2
No. 167 Bromochloroacetylene C_2BrCl
No. 168 Chloroiodoacetylene C_2ClI
No. 169 Bromoiodoacetylene C_2BrI

C_2–six–atomic molecules

No. 170 Trifluoroacetonitrile CF_3CN
No. 171 trans–1,2–Difluoroethylene CHFCHF
No. 172 trans–1,2–Difluoroethylene–d_1 CHFCDF
No. 173 trans–1,2–Difluoroethylene–d_2 CDFCDF
No. 174 Glyoxal $C_2H_2O_2$
No. 175 Glyoxal–d_1 C_2HDO_2
No. 176 Glyoxal–d_2 $C_2D_2O_2$

C_2–seven–atomic molecules

No. 177 Acetyl fluoride CH_3COF
No. 178 Acetyl fluoride–d_3 CD_3COF

C_2–nine–atomic molecules

No. 179 Dimethylzinc CH_3ZnCH_3
No. 180 Dimethylzinc–d_6 CD_3ZnCD_3
No. 181 Dimethylcadmium CH_3CdCH_3
No. 182 Dimethylcadmium–d_6 CD_3CdCD_3
No. 183 Dimethylmercury CH_3HgCH_3
No. 184 Dimethylmercury–d_6 CD_3HgCD_3

C_2–ten–atomic molecules

No. 185 Azomethane CH_3NNCH_3
No. 186 Azomethane–d_6 CD_3NNCD_3

C_3–five–atomic molecules

No. 187 Carbon suboxide C_3O_2
No. 188 Carbon subsulfide C_3S_2
No. 189 Chloro cyanoacetylene ClCCCN
No. 190 Bromo cyanoacetylene BrCCCN
No. 191 Iodo cyanoacetylene ICCCN

C_3–seven–atomic molecules

No. 192 Chloropropadiene CH_2CCHCl
No. 193 Bromopropadiene CH_2CCHBr
No. 194 Iodopropadiene CH_2CCHI
No. 195 Trifluoropropyne CF_3CCH
No. 196 Trifluoropropyne–d CF_3CCD
No. 197 1–Chloro–3,3,3–trifluoropropyne CF_3CCCl
No. 198 1–Bromo–3,3,3–trifluoropropyne CF_3CCBr
No. 199 1–Iodo–3,3,3–trifluoropropyne CF_3CCI
No. 200 Propargyl fluoride $CHCCH_2F$
No. 201 Propargyl chloride $CHCCH_2Cl$
No. 202 Propargyl bromide $CHCCH_2Br$
No. 203 Propargyl iodide $CHCCH_2I$

C_4–six–atomic molecules

No. 204 Chlorodiacetylene ClCCCCH
No. 205 Bromodiacetylene BrCCCCH
No. 206 Iododiacetylene ICCCCH

C_4–fourteen–atomic molecules

No. 207 1,4–Dioxane $C_4H_8O_2$

C_5–eight–atomic molecules

No. 208 Diethynyl ketone $(HC{\equiv}C)_2CO$

C_6–eight–atomic molecules

No. 209 Dicyanodiacetylene NCCCCCCN

C_6–thirteen–atomic molecules

No. 210 Hexacarbonylchromium(0) $Cr(^{12}C^{16}O)_6$
No. 211 Hexacarbonylmolybdenum(0) $Mo(^{12}C^{16}O)_6$
No. 212 Hexacarbonyltungsten(0) $W(^{12}C^{16}O)_6$

No. 1 Krypton difluoride KrF_2
Symmetry $D_{\infty h}$ **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	Sym. stretch.	449 B	ia	449	
π_u	ν_2	Bend.	233 B	232.6 S	ia	
σ_u^+	ν_3	Antisym. stretch.	590 A	589.89 VS	ia	

References
[1] IR.R. H. H. Classen, G. L. Goodman, J. G. Malm, and F. Schreiner, J. Chem. Phys. **42**, 1229 (1965).
[2] IR. C. Murchison, S. Reichman, D. Anderson, J. Overend, and F. Schreiner, J. Amer. Chem. Soc. **90**, 5690 (1968).

No. 2 Nitrogen dioxide $^{14}NO_2$
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1318 B	1318 W		
	ν_2	Bend.	750 A	749.650 S		
b_1	ν_3	Antisym. stretch.	1618 B	1617.8 VS		

References
[1] IR. E. T. Arakawa and A. H. Nielsen, J. Mol. Spectry. **2**, 413 (1958).
[2] IR. J. W. Keller and A. H. Nielsen, J. Chem. Phys. **29**, 252 (1958).
[3] IR. S. C. Hurlock, K. N. Rao, L. A. Weller, and P. K. L. Yin, J. Mol. Spectry. **48**, 372 (1973).

No. 3 Nitrogen dioxide $^{15}NO_2$
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1306 B	1306 W		
	ν_2	Bend.	740 B	740.2 S		
b_1	ν_3	Antisym. stretch.	1580 B	1580.3 VS		

Reference
[1] IR. E. T. Arakawa and A. H. Nielsen, J. Mol. Spectry. **2**, 413 (1958).

No. 4 Ozone $^{16}O_3$
Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1103 A	1103.157 VW		
	ν_2	Bend.	701 B	701.42 W		
b_1	ν_3	Antisym. stretch.	1042 A	1042.096 S		

References

[1] IR. S. A. Clough and F. X. Kneizys, J. Chem. Phys. **44**, 1855 (1966).
[2] IR. D. J. McCaa and J. H. Shaw, J. Mol. Spectry. **25**, 374 (1968).
[3] IR. J. L. Brumant, A. Barve, and P. Jouve, Comptes Rendus **B268**, 459 (1969).

No. 5 Ozone $^{18}O_3$
Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Xe Matrix)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1038 C	1038 W		
	ν_2	Bend.	660 C	660 W		
b_1	ν_3	Antisym. stretch.	974 C	974 S		

References

[1] IR. L. Brewer and J. Ling–Fai Wang, J. Chem. Phys. **56**, 759 (1972).
[2] IR.Th. M. Spoliti, S. N. Cesaro, and B. Mariti, J. Chem. Phys. **59**, 985 (1973).

No. 6 Water $H_2{}^{18}O$
Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	3650 A	3649.68		
	ν_2	Bend	1588 A	1588.275		
b_1	ν_3	Antisym. stretch.	3742 A	3741.58		

References

[1] IR. W. S. Benedict, Mem. Soc. Roy. Sci. Liege, **18**, 557 (1957).
[2] IR. P. E. Fraley, K. N. Rao, and L. H. Jones, J. Mol. Spectry. **29**, 312 (1969).
[3] IR. J. G. Williamson, K. N. Rao, and L. H. Jones, J. Mol. Spectry. **40**, 372 (1971).

No. 7 Sulfur dioxide $S^{18}O_2$
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹	
a_1	ν_1	Sym. stretch.	1101 B	1100.65		
	ν_2	Bend.	497 B	496.7		
b_1	ν_3	Antisym. stretch.	1318 B	1317.9		

Reference
[1] IR. A. Barbe and P. Jauve, J. Mol. Spectry. **38**, 273 (1971).

No. 8 Sulfur dichloride SCl_2
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a_1	ν_1	Sym. stretch.	525 D	525 VS	514 (10), p	
	ν_2	Bend.	208 B		208 (5), p	
b_1	ν_3	Antisym. stretch.	535 D		535 (1)	

References
[1] R. H. Stammerich, R. Forneris, and K. Sone, J. Chem. Phys. **23**, 972 (1955).
[2] IR. G. M. Barrow, Can. J. Chem. **59**, 987 (1955).
[3] IR. Y. Morino, Y. Murata, T. Ito, and J. Nakamura, J. Phys. Soc. Japan **17**, Supplement B–II, 37 (1962

No. 9 Germanium (II) chloride $GeCl_2$
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Ar Matrix)	cm⁻¹ (Gas)	
a_1	ν_1	Sym. stretch.	399 C	399	399 p	
	ν_2	Bend.	159 C		159 p	
b_1	ν_3	Antisym. stretch.	374 D	374	362 dp (Ar Matrix)	

References
[1] R. I. R. Beattie and R. O. Perry, J. Chem. Soc. **A1970**, 2429.
[2] IR. L. Andrews and D. L. Frederick, J. Amer. Chem. Soc. **92**, 775 (1970).
[3] R. G. A. Ozin and A. Vander Voet, J. Chem. Phys. **56**, 4768 (1972).

No. 10 Tin (II) fluoride SnF_2
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1}	
a_1	ν_1	Sym. stretch.	593 D	592.7		
	ν_2	Bend.	197 D	197		
b_1	ν_3	Antisym. stretch.	571 D	570.9		

Reference
[1] IR. R. H. Hauge, J. W. Hastie, and J. L. Margrave, J. Mol. Spectry. **45**, 420 (1973).

No. 11 Tin (II) chloride $SnCl_2$
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	352 C	354	352 p	
	ν_2	Bend.	120 C		120 p	
b_1	ν_3	Antisym. stretch.	334 D	334	332 (Ar Matrix)	

References
See No. 9($GeCl_2$).

No. 12 Tin (II) bromide $SnBr_2$
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	244 D		244 (Ar Matrix)	
	ν_2	Bend.	80 C		80	
b	ν_3	Antisym. stretch.	231 D		231 (Ar Matrix)	

References
See No. 9($GeCl_2$).

No. 13 Lead (II) fluoride PbF_2
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1}	
a_1	ν_1	Sym. stretch.	531 D	531.2		
	ν_2	Bend.	165 D	165		
b_1	ν_3	Antisym. stretch.	507 D	507.2		

Reference
See No. 10(SnF_2).

No. 14 Lead (II) chloride $PbCl_2$
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	314 C	322	314 p	
	ν_2	Bend.	99 C		99 p	
b_1	ν_3	Antisym. stretch.	299 D	299	300 dp (Ar Matrix)	

References
See No. 9($GeCl_2$).

No. 15 Nitrosyl fluoride $^{16}O^{14}NF$
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO stretch.	1844 B	1843.5 VS		
	ν_2	NF stretch.	766 B	765.8 VS		
	ν_3	Bend.	520 C	519.9 VS		

References
[1] IR. P. J. H. Woltz, E. A. Jones, and A. H. Nielsen, J. Chem. Phys. **20**, 378 (1952).
[2] IR. D. W. Magnuson, J. Chem. Phys. **20**, 380 (1952).
[3] IR. L. H. Jones, L. B. Asprey, and R. R. Ryan, J. Chem. Phys. **47**, 3371 (1967).

No. 16 Nitrosyl fluoride $^{16}O^{15}NF$
Symmetry C_s Symmetry number σ = 1

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO stretch.	1812 C	1811.8 VS		
	ν_2	NF stretch.	749 C	748.7 VS		
	ν_3	Bend.	517 C	517.4 VS		

Reference

[1] IR. L. H. Jones, L. B. Asprey, and R. R. Ryan, J. Chem. Phys. **47**, 3371 (1967).

No. 17 Nitrosyl fluoride $^{18}O^{14}NF$
Symmetry C_s Symmetry number σ = 1

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO stretch.	1796 C	1795.6 VS		
	ν_2	NF stretch.	758 C	757.8 VS		
	ν_3	Bend.	511 C	511.3 VS		

Reference

See No. 16($^{16}O^{15}NF$).

No. 18 Nitrosyl fluoride $^{18}O^{15}NF$
Symmetry C_s Symmetry number σ = 1

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO stretch.	1763 C	1763.0 VS		
	ν_2	NF stretch.	740 C	740.4 VS		
	ν_3	Bend.	509 C	509.3 VS		

Reference

See No. 16($^{16}O^{15}NF$).

No. 19 Nitrosyl chloride $^{16}O^{14}NCl$
Symmetry C_S Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹	
a'	ν_1	NO stretch.	1800 C	1799.7 VS		
	ν_2	NCl stretch.	596 C	595.8 VS		
	ν_3	Bend.	332 C	331.9 VS		

References

[1] IR. W. G. Burns, and H. J. Bernstein, J. Chem. Phys. **18**, 1669 (1950).
[2] IR. A. G. Pulford and A. Walsh, Trans. Faraday Soc. **47**, 347 (1951).
[3] IR. W. H. Eberhardt and T. G. Burke, J. Chem. Phys. **20**, 529 (1952).
[4] IR. L. Landau and W. H. Fletcher, J. Mol. Spectry. **4**, 276 (1960).
[5] IR. L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Chem. Phys. **49**, 581 (1968).

No. 20 Nitrosyl chloride $^{16}O^{15}NCl$
Symmetry C_S Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹	
a'	ν_1	NO stretch.	1769 C	1768.9 VS		
	ν_2	NCl stretch.	582 C	581.7 VS		
	ν_3	Bend.	330 C	329.9 VS		

References

[1] IR. L. Landau and W. H. Fletcher, J. Mol. Spectry. **4**, 276 (1960).
[2] IR. L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Chem. Phys. **49**, 581 (1968).

No. 21 Nitrosyl chloride $^{18}O^{14}NCl$
Symmetry C_S Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹	
a'	ν_1	NO stretch.	1751 C	1752.7 VS 1749.0 VS		FR($3\nu_2$)
	ν_2	NCl stretch.	588 C	588.4 VS		
	ν_3	Bend.	325 C	324.9 VS		

Reference

[1] IR. L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Chem. Phys. **49**, 581 (1968).

No. 22 Nitrosyl chloride $^{18}O^{15}NCl$
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO stretch.	1721 C	1720.6 VS		
	ν_2	NCl stretch.	574 C	573.9 VS		
	ν_3	Bend.	323 C	323.2 VS		

Reference

See No. 21($^{18}O^{14}NCl$)

No. 23 Nitrosyl bromide $^{16}O^{14}NBr$
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO stretch.	1799 C	1799.0 VS		
	ν_2	NBr stretch.	542 C	542.0 VS		
	ν_3	Bend.	266 C	266.4 S		

References

[1] IR. W. G. Burns and H. J. Bernstein, J. Chem. Phys. **18**, 1669 (1950).
[2] IR. J. Laane, L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Mol. Spectry. **30**, 485 (1969).

No. 24 Nitrosyl bromide $^{16}O^{15}NBr$
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO stretch.	1768 C	1768.3 VS		
	ν_2	NBr stretch.	528 D	527.8 VS		
	ν_3	Bend.	264 C	264 S		

Reference

[1] IR. J. Laane, L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Mol. Spectry. **30**, 485 (1969).

No. 25 Nitrosyl bromide $^{18}O^{15}NBr$
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO stretch.	1720 C	1719.5 VS		
	ν_2	NBr stretch.	522 C	521.5 VS		
	ν_3	Bend.	257 C	257.0 S		

Reference

See No. 24($^{16}O^{15}NBr$).

No. 26 Hypofluorous acid HOF
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (N_2 Matrix)	cm^{-1}	
a'	ν_1	OH stretch.	3537 C	3537.1		
	ν_2	OF stretch.	1393 C	1393.0		
	ν_3	Bend.	886 C	886.0		

References

[1] IR. P. N. Noble and G. C. Pimentel, Spectrochim. Acta **24A**, 797 (1968).
[2] IR. J. A. Golb, H. H. Claassen, M. H. Studier, and E. H. Appklman, Spectrochim. Acta **28A**, 65 (1972).

No. 27 Hypochlorous acid HOCl
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OH stretch.	3609 A	3609 M		
	ν_2	Bend.	1242 C	1242 S		
	ν_3	OCl stretch.	725 C	725 M		

References

[1] IR. K. Hedberg and R. M. Badger, J. Chem. Phys. **19**, 508 (1951).
[2] IR. R. A. Ashby, J. Mol. Spectry. **23**, 439 (1967).
[3] IR. I. Schwager and A. Arkell, J. Amer. Chem. Soc. **89**, 6006 (1967).
[4] IR. R. A. Ashby, J. Mol. Spectry. **40**, 639 (1971).

No. 28 Hypochlorous acid-d DOCl
Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OD stretch.	2666 B	2666 M		
	ν_2	Bend.	911 C	911 S		
	ν_3	OCl stretch.	739 C	739 M		

References
[1] IR. K. Hedberg and R. M. Badger, J. Chem. Phys. **19**, 508 (1951).
[2] IR. R. A. Ashby, J. Mol. Spectry. **23**, 439 (1967).

No. 29 Thionitrosyl-S-fluoride NSF
Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NS stretch.	1372 C	1372 VS		
	ν_2	SF stretch.	640 C	640 VS		
	ν_3	Bend.	366 C	366 S		

References
[1] IR. H. Richert and O. Glemser, Z. Anorg. Alleg. Chem. **307**, 328 (1961).
[2] IR. I. Schwager and A. Arkell, J. Amer. Chem. Soc. **89**, 6006 (1967).

No. 30 Thionitrosyl-S-chloride NSCl
Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NS stretch.	1325 C	1325		
	ν_2	SCl stretch.	414 C	414		
	ν_3	Bend.	273 D			OC($\nu_2+\nu_3$, $2\nu_3$).

Reference
[1] IR. A. Müller, G. Nagarajan, O. Glemser, S. F. Cyvin, and J. Wegener, Spectrochim. Acta **23A**, 2683 (1967).

No. 31 Boron trifluoride $^{10}BF_3$
Symmetry D_{3h} **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	Sym. stretch.	888 B	ia	888 VS	
a_2''	ν_2	Op–deform.	719 A	719.3 S	ia	
e'	ν_3	Deg. stretch.	1503 A	1502.5 S	1481 VW	
	ν_4	Deg. deform.	482 B	482.0 M	482 W, b	

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No. 32 Boron trifluoride $^{11}BF_3$
Symmetry D_{3h} **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	Sym. stretch.	888 B	ia	888 VS	
a_2''	ν_2	Op–deform.	691 A	691.2 S	ia	
e'	ν_3	Deg. stretch.	1449 B	1449 S	1448 VW	
	ν_4	Deg. deform.	480 B	480.4 M	482 b	

References

See No. 31($^{10}BF_3$).

No. 33 Sulfur trioxide SO_3
Symmetry D_{3h} **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	Sym. stretch.	1065 B	ia	1065 VS, p	
a_2''	ν_2	Op deform.	498 B	497.55 M	ia	
e'	ν_3	Deg. stretch.	1391 A	1391.3 VS	1390 W	
	ν_4	Deg. deform.	530 B	530.2 S	528 W	

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[1] R. H. Gerding and W. J. Nijverd, Rec. Trav. Chim. **59**, 1206 (1940).
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No. 34 Ammonia–t_3 NT_3
Symmetry C_{3V} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	2014 A	2014.1		
	ν_2	Sym. deform.	657 B	656.4 s[a] 657.2 a[a]		
e	ν_3	Deg. stretch.	2185 A	2184.8		
	ν_4	Deg. deform.	996 A	996.3		

[a] "s" and "a" refer to symmetric and antisymmetric levels [1].

References

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[2] IR. L. H. Jones, W. W. Brim, and K. N. Rao, J. Mol. Spectry. **11**, 389 (1963).

No. 35 Nitrogen trifluoride $^{15}NF_3$
Symmetry C_{3V} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1009 A	1008.93		
	ν_2	Sym. deform.	645 B	644.84		
e	ν_3	Deg. stretch.	886 A	886.34		
	ν_4	Deg. deform.	492 B	492.02		

References
[1] MW. M. Otake, C. Matsumura, and Y. Morino, J. Mol. Spectry. **28**, 316 (1968).
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No. 36 Aluminum trichloride $AlCl_3$
Symmetry C_{3V} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	375 C	380.2	375 p	
	ν_2	Sym. deform.	183 C	182.8		
e	ν_3	Deg. stretch.	595 C	594.7		
	ν_4	Deg. deform.	150 C	149.2	150	

References
[1] IR. W. Klemperer, J. Chem. Phys. **24**, 353 (1956).
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No. 37 Phosphorus triiodide PI_3
Symmetry C_{3V} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (CS_2,C_6H_6, CH_2Cl_2 soln.)	cm^{-1} C_6H_6, CCl_4 soln.)	
a_1	ν_1	Sym. stretch.	303 D	306 M	303 (3) p	
	ν_2	Sym. deform.	111 D	112 VW	111 (7) p	
e	ν_3	Deg. stretch.	325 D	328 VS	325 (1b) dp	
	ν_4	Deg. deform.	79 D	80 VW, b	79 (10) dp	

References
[1] R. R. H. Stammreich, R. Forneris, and Y. Tavares, J. Chem. Phys. **25**, 580 (1956).
[2] IR. S. G. Frankiss, F. A. Miller, H. Stammreich and Th. T. Sans, Spectrochim. Acta **23A**, 543 (1967).

No. 38 Arsenic trifluoride AsF_3
Symmetry C_{3V} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.	741 A	740.5 S	707 (10)	
	ν_2	Sym. deform.	337 B	336.5 M	341 (2)	
e	ν_3	Deg. stretch.	702 B	702.2 S	644 (9)	
	ν_4	Deg. deform.	262 B	262.3 M	274 (4)	

References
[1] R. D. M. Yost and J. E. Sherborne, J. Chem. Phys. **2**, 125 (1934).
[2] IR. L. C. Hoskins and R. C. Lord, J. Chem. Phys. **43**, 155 (1965).
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[4] IR.Th. L. C. Hoskins, J. Chem. Phys. **45**, 4594 (1966).
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[7] Th. S. Reichman, D. F. Smith, Jr. and J. Overend, Spectrochim. Acta **26A**, 927 (1970).

No. 39 Arsenic triiodide AsI_3
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Solid)	cm^{-1} ($CHBr_3$,CS_2 soln.)	
a_1	ν_1	Sym. stretch.	219 C	225.7	218.5 p	
	ν_2	Sym. deform.	94 C	101.6	94 p	
e	ν_3	Deg. stretch.	224 C	201.2 VVS,b	223.5 dp	
	ν_4	Deg. deform.	71 C	73.6	71 dp	

References

[1] R. R. H. Stammreich, R. Forneris, and Y. Tavares, J. Chem. Phys. **25**, 580 (1956).
[2] IR. T. R. Marley and D. A. Williams, Spectrochim. Acta **21**, 1773 (1968).
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No. 40 trans-1,2-Difluorodiazine N_2F_2
Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_g	ν_1	NN stretch.	1523 C	ia	1523 (2)	
	ν_2	NF stretch.	1018 C	ia	1018 (5)	
	ν_3	FNN deform.	603 C	ia	603 (10)	
a_u	ν_4	Torsion	364 B	363.5 M	ia	
b_u	ν_5	NF stretch.	991 A	991.01 VS	ia	
	ν_6	FNN deform.	423 C	423 M	ia	

References

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[2] IR.R. S-T. King and J. Overend, Spectrochim. Acta **22**, 689 (1966).
[3] IR. S-T. King and J. Overend, Spectrochim. Acta **23A**, 2875 (1967).
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No. 41 Nitryl fluoride $F^{14}NO_2$
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	NO_2 s-stretch.	1310 B	1309.6 VS		
	ν_2	NF stretch.	822 B	822.4 VS		
	ν_3	NO_2 scis.	568 C	567.8 S		
b_1	ν_4	NO_2 a-stretch.	1792 B	1791.5 VS		
	ν_5	NO_2 rock.	560 C	559.6 S		
b_2	ν_6	Op-deform.	742 B	742.0 M		

References

[1] IR. R. E. Dodd, J. A. Roufe, and L. A. Woodward, Trans. Farad. Soc. **52**, 145 (1956).
[2] IR. D. L. Bernitt, R. H. Miller, and I. C. Hisatsune , Spectrochim. Acta **22A**, 237 (1967).
[3] Th. T. Tanaka and Y. Morino, J. Mol. Spectry. **32**, 430 (1969).

No. 42 Nitryl fluoride $F^{15}NO_2$
Symmetry C_{2V} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	NO_2 s-stretch.	1298 B	1298.0 VS		
	ν_2	NF stretch.	809 B	808.5 VS		
	ν_3	NO_2 scis.	567 C	567.1 S		
b_1	ν_4	NO_2 a-stretch.	1751 B	1750.5 VS		
	ν_5	NO_2 rock.	559 C	558.9 S		
b_2	ν_6	Op-deform.	722 B	722.0 M		

References

See No. 41($F^{14}NO_2$).

No. 43 Nitryl chloride $Cl^{14}NO_2$
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	NO_2 s-stretch.	1286 C	1318.5 S		
				1267.1 VS		FR($2\nu_6$).
	ν_2	NCl stretch.	793 B	792.6 VS		
	ν_3	NO_2 scis.	370 C	369.6 VS		
b_1	ν_4	NO_2 a-stretch.	1685 B	1684.6 VS		
	ν_5	NO_2 rock.	408 C	408.1 VW		
b_2	ν_6	Op-deform.	652 C	652.3 M		

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[1] IR. R. Ryason and M. K. Wilson, J. Chem. Phys. **22**, 2000 (1954).
[2] IR. D. L. Bernitt, R. H. Miller, and I. C. Hisatsune , Spectrochim. Acta **23A**, 237 (1967).

No. 44 Nitryl chloride $Cl^{15}NO_2$
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	NO_2 s-stretch.	1286 D	1318.5 S		
				1267.1 VS		FR($2\nu_6$).
	ν_2	NCl stretch.	793 B	792.6 VS		
	ν_3	NO_2 scis.	370 C	369.6 VS		
b_1	ν_4	NO_2 a-stretch.	1685 B	1684.6 VS		
	ν_5	NO_2 rock.	408 C	408.1 VW		
b_2	ν_6	Op-deform.	652 C	652.3 M		

References

See No. 43($Cl^{14}NO_2$).

No. 45 Chlorine trifluoride ClF_3
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	ClF stretch.	752 C	751 S	752.1 S, p	
	ν_2	ClF_2 s-stretch.	529 C	530 M	529.3 VS, p	
	ν_3	ClF_2 ip-deform.	328 C	328 S	337 W, p 321	OV(ν_6).
b_1	ν_4	ClF_2 a-stretch.	702 C	702 VS		
	ν_5	ClF_2 ip-deform.	442 C	442 W	431 W, dp	
b_2	ν_6	ClF_2 op-deform.	328 D	328 S		OV(ν_3).

References
[1] IR.R. H. Selig, H. H. Claassen, and J. H. Holloway, J. Chem. Phys. **52**, 3517 (1970).
[2] Th. K. Ramaswamy and P. Muthusbramanian, J. Mol. Structure **9**, 193 (1971).

No. 46 Bromine trifluoride BrF_3
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	BrF stretch.	675 C	675 S	675 S, p	
	ν_2	BrF_2 s-stretch.	552 C	552 W	552 VS, p	
	ν_3	BrF_2 ip-deform.	242 C	242 S	233 W, p	OV(ν_6).
b_1	ν_4	BrF_2 a-stretch.	614 C	614 VS	612 VW	
	ν_5	BrF_2 ip-deform.	350 C	350 VW		
b_2	ν_6	BrF_2 op-deform.	242 D	242 S		OV(ν_3).

References
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[2] IR. K. O. Christe, E. C. Curtis, and D. Pilipovich, Spectrochim. Acta **27A**, 931 (1971).
[3] Th. K. Ramaswamy and P. Muthusbramanian, J. Mol. Structure **9**, 193 (1971).

No. 47 Hydrogen peroxide H_2O_2

Symmetry C_2 Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a	ν_1	OH stretch.	3599 B	3599.2	3364 p	
	ν_2	OH bend.	1402 E		1402 p	
	ν_3	OO stretch.	877 C	877	880 p	
	ν_4	Torsion	371 B	370.7		
			243 C	242.8		
b	ν_5	OH stretch.	3608 B	3607.9		
	ν_6	OH bend.	1266 D	1266		

References

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No. 48 Hydrogen persulfide H_2S_2

Symmetry C_2 Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a	ν_1	SH stretch.	2556 A	2555.78	2509 (2), dp	
	ν_2	SH bend.	883 D		883 (2), dp	
	ν_3	SS stretch.	509 D		509 (9)	
	ν_4	Torsion	416 B	416		
b	ν_5	SH stretch.	2559 A	2558.64		
	ν_6	SH bend.	886 C	886		

References

[1] IR. M. K. Wilson and R. M. Badger, J. Chem. Phys. **17,** 1232 (1949).
[2] R. F. Fehér, W. Laue, and G. Winkhaus, Z. Anorg. Allg. Chem. **288**, 113 (1956).
[3] IR. R. L. Redington, J. Mol. Spectry. **9.** 469 (1962).
[4] IR. B. P. Winnwisser, J. Mol. Spectry. **36,** 414 (1970).

No. 49 Difluoro disulphane F_2S_2
Symmetry C_2 **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a	ν_1	SF stretch.	717 B	717.0		
	ν_2	SS stretch.	615 B	614.6	623 p	
	ν_3	SF bend.	320 B	319.8	322 p	
	ν_4	Torsion	183 C	182.5	193 p	
b	ν_5	SF stretch.	681 B	680.8	683	
	ν_6	SF bend.	301 C	301	297 dp	

References

[1] IR. F. Seel and R. Budenz, Chem. Ber. **98**, 251 (1965).
[2] IR.R. R. D. Brown and G. P. Pez, Spectrochim. Acta **26A**, 1375 (1970).

No. 50 Hydrazoic acid HN_3
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NH stretch.	3336 B	3336 M		
	ν_2	N≡N stretch.	2140 B	2139.8 VS		
	ν_3	NH bend.	1264 B	1263.7 M		
	ν_4	N–N stretch.	1151 B	1150.5 VS		
	ν_5	NNN bend.	534 B	534.2 W		
a''	ν_6	NNN bend.	607 B	607.0 VW		

References

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[4] IR. D. M. Levine and D. A. Dows, J. Chem. Phys. **46**, 1168 (1967).

No. 51 Hydrazoic acid DN_3
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	ND stretch.	2478 B	2478 M		
	ν_2	N≡N stretch.	2112 C	2112 VS		FR($\nu_3+\nu_4$).
	ν_3	ND bend.	954 B	953.8 S		
	ν_4	N–N stretch.	1184 B	1183.7 M		
	ν_5	NNN bend.	492 B	492.2 W		
a''	ν_6	NNN bend.	588 B	588.4 VW		

References
See No. 50(NH_3).

No. 52 Difluoroamine NF_2H
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NH stretch.	3193 C	3193 W		
	ν_2	NH bend.	1307 B	1307 S		
	ν_3	NF_2 s-stretch.	972 B	972 S		
	ν_4	NF_2 scis.	500 C	500 M		
a''	ν_5	NH bend.	1424 B	1424 S		
	ν_6	NF_2 a-stretch.	888 C	888 VS		

Reference
[1] IR. J. J. Comeford, D. E. Mann, J. L. Schoen, and D. R. Lide, Jr., J. Chem. Phys. **38**, 461 (1963).

No. 53 Chlorodifluoroammonia $NClF_2$
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NF_2 s-stretch.	930 C	930.2		
	ν_2	NCl stretch.	697 C	696.9		
	ν_3	NF_2 deform.	556 C	555.5		
	ν_4	NClF s-deform.	377 C	377		
a''	ν_5	NF_2 a-stretch.	855 C	855.4		
	ν_6	NClF a-deform.	382 D	382[a]		

[a] An average of two splitting bands.

References
[1] IR. R. Ettinger, J. Chem. Phys. **38**. 2427 (1963).
[2] IR. J. J. Comeford, J. Chem. Phys. **45**, 3463 (1966).

No. 54 Dichlorofluoroammonia NCl_2F
Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NF stretch.	825 C	825 S		
	ν_2	NCl_2 s-stretch.	615 C	615 M		
	ν_3	NFCl s-deform.	409 C	409 W		
	ν_4	NCl_2 deform.	274 C	274 W		
a''	ν_5	NCl_2 a-stretch.	692 C	692 S		
	ν_6	NFCl a-deform.	344 C	344 M		

References
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[2] IR. R. P. Hirschmann, L. R. Anderson, D. F. Harnish, and W. B. Fox, Spectrochim. Acta **24A**, 1267 (1968).

No. 55 Thionyl fluoride SOF_2
Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a'	ν_1	SO stretch.	1333 D	1340.8 S	1339.3 VS	
				1330.9 S	1329.9 VS	FR($\nu_2+\nu_3$).
	ν_2	SF_2 s-stretch.	808 B	808.2 VS	808.3 VS	
	ν_3	OSF deform.	530 B	530.4 M	529.6 S	
	ν_4	SF_2 scis.	378 D	377.8 W	379.5 W (liquid)	
a''	ν_5	SF_2 a-stretch.	747 C	747.0 VS	746.8 W	
	ν_6	OSF deform.	393 D	392.5 W	398.6 M (liquid)	

References
[1] IR. J. K. O'Loane and M. K. Wilson, J. Chem. Phys. **23**, 1313 (1955).
[2] R. P. Bender and J. M. Wood, Jr., J. Chem. Phys. **23**, 1316 (1955).
[3] IR. F. Seel and R. Budenz. Chem. Ber. **98**, 251 (1965).
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No. 56 Thionyl chloride $SOCl_2$
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a'	ν_1	SO stretch.	1251 C	1251 VS	1230 W, p	
	ν_2	SCl_2 s-stretch.	492 C	492 VS	490 M, p	
	ν_3	OSCl deform.	344 D		344 S, p	
	ν_4	SCl_2 scis.	194 D		194 M, p	
a''	ν_5	SCl_2 a-stretch.	455 C	455 VS	445 W, dp	
	ν_6	OSCl deform.	284 D		284 M, dp	

References

[1] R. R. Vogel–Hogler, Acta. Phys. Austriaca **1**, 323 (1948).
[2] R. C. A. McDowell, Trans. Faraday Soc. **49**, 371 (1953).
[3] IR. D. E. Martz and R. T. Lagemann, J. Chem. Phys. **22**, 1193 (1954).
[4] R. G. Allen and C. A. McDowell, J. Chem. Phys. **23**, 209 (1955).
[5] Th. A. Mueller and G. Nagarajan, Z. Phys. Chem. (Leipzig) **235**, 57 (1967).
[6] Th. K. Ramaswamy and S. Jayaraman, J. Mol. Structure **7**, 470 (1971).

No. 57 Thionyl bromide $SOBr_2$
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹	cm⁻¹ (Liquid)	
a'	ν_1	SO stretch.	1121 D	1121 (2) p		
	ν_2	SBr s-stretch.	405 D		405 (7) p	
	ν_3	OSBr deform.	267 D		267 (10) p	
	ν_4	SBr_2 scis.	120 D		120 (10) p	
a''	ν_5	SBr_2 a-stretch.	379 D		379 (5) dp	
	ν_6	OSBr deform.	223 D		223 (7) dp	

Reference

[1] R. H. Stammereich, R. Forneris, and Y. Tavares, J. Chem. Phys. **25**, 1277 (1956).

No. 58 Titanium tetrachloride $TiCl_4$

Symmetry T_d **Symmetry number $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	389 B	ia, 388[a]	389	
e	ν_2	Deg. deform.	114 B	ia, 119[a]	114	
f_2	ν_3	Deg. stretch.	498 C	498.5	498	
	ν_4	Deg. deform.	136 C	136	136	

[a] Estimated from combination bands.

References

[1] IR. N. J. Hawkins and D. R. Carpenter, J. Chem. Phys. **23**, 1700 (1955).
[2] IR. H. Bürger and A. Ruoff, Spectrochim. Acta **24A**, 1863 (1968).
[3] R. R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

No. 59 Titanium tetrabromide $TiBr_4$

Symmetry T_d **Symmetry number $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Liquid)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	232 B	ia	231.5	
e	ν_2	Deg. deform.	69 B	ia	68.5	
f_2	ν_3	Deg. stretch.	393 C	383 VS	393	
	ν_4	Deg. deform.	88 C		88	

References

[1] IR.R. F. A. Miller and G. L. Carlson, Spectrochim. Acta **16**, 6 (1960).
[2] R. R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

No. 60 Titanium tetraiodide TiI_4

Symmetry T_d **Symmetry number $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (C_6H_{12} soln.)	cm^{-1} (C_6H_{12} soln.)	
a_1	ν_1	Sym. stretch.	162 D	ia	162 VS, p	
e	ν_2	Deg. deform.	51 D	ia	51 M, dp	
f_2	ν_3	Deg. stretch.	322 D	322 VS	324 M, dp	
	ν_4	Deg. deform.	67 D	67 M		

Reference

[1] IR. R. R. J. H. Clark and C. J. Willis, J. Chem. Soc. A **1971**, 838.

No. 61 Zirconium tetrachloride $ZrCl_4$
Symmetry T_d **Symmetry number σ = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	377 B	ia, 388[a]	377 VS, p	
e	ν_2	Deg. deform.	98 B	ia, 102[a]	98	
f_2	ν_3	Deg. stretch.	418 C	421	418 VW	
	ν_4	Deg. deform.	113 C	112[a]	113	

[a] Estimated from combination bands.

References

[1] IR. J. K. Wilmshurst, J. Mol. Spectry. **5**, 343 (1960).
[2] IR. A. Büchler, J. B. Berkowitz–Mattuck, and D. H. Dugre, J. Chem. Phys. **34**, 2202 (1961).
[3] R. R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

No. 62 Zirconium tetrabromide $ZrBr_4$
Symmetry T_d **Symmetry number σ = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	223 B	ia	222.5	
e	ν_2	Deg. deform.	60 B	ia	60	
f_2	ν_3	Deg. stretch.	315 C		315	
	ν_4	Deg. deform.	72 C		72	

Reference

[1] R. R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

No. 63 Zirconium tetraiodide ZrI_4
Symmetry T_d **Symmetry number σ = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	158 B	ia	158	
e	ν_2	Deg. deform.	43 B	ia	43	
f_2	ν_3	Deg. stretch.	254 C		254	
	ν_4	Deg. deform.	55 C		55	

Reference

See No. 62($ZrBr_4$).

No. 64 Ruthenium tetroxide RuO_4
Symmetry T_d **Symmetry number σ = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a_1	ν_1	Sym. stretch.	885 C	ia	885.3 S	
					(Gas)	
e	ν_2	Deg. deform.	322 C	ia	322.4 M	
f_2	ν_3	Deg. stretch.	921 C	921.0	912.9 W	
	ν_4	Deg. deform.	336 C	336.0	333 W	

References

[1] IR. R. E. Dodd, Trans. Faraday Soc. **55**, 1480 (1959).
[2] IR. M. H. Ortner, J. Chem. Phys. **34**, 559 (1961).
[3] R. G. Davidson, N. Logan, and A. Morris, Chem. Commun. **1968**, 1044.
[4] R. W. P. Griffith, J. Chem. Soc. **A1968**, 1663.
[5] IR. A. Müller and B. Krebs, J. Mol. Spectry. **26**, 136 (1968).
[6] IR.R. I. W. Levin and S. Abramowitz, J. Chem. Phys. **50**, 4860 (1969).
[7] Th. R. S. McDowell, J. Chem. Phys. **53**, 4407 (1970).
[8] IR.R. R. S. McDowell, L. B. Aspery and L. C. Hoskins, J. Chem. Phys. **56**, 5712 (1972).

No. 65 Hafnium tetrachloride $HfCl_4$
Symmetry T_d **Symmetry number σ = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Gas)	
a_1	ν_1	Sym. stretch.	382 B	ia	382	
e	ν_2	Deg. deform.	102 B	ia	101.5	
f_2	ν_3	Deg. stretch.	390 C	393	390	
	ν_4	Deg. deform.	112 C		112	

References

[1] IR. A. Büchler, J. B. Berkowitz–Mattuck, and D. H. Dugre, J. Chem. Phys. **34**, 2202 (1961).
[2] R. R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

No. 66 Hafnium tetrabromide $HfBr_4$
Symmetry T_d **Symmetry number σ = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹	cm⁻¹ (Gas)	
a_1	ν_1	Sym. stretch.	236 B	ia	235.5	
e	ν_2	Deg. deform.	63 B	ia	63	
f_2	ν_3	Deg. stretch.	273 C		273	
	ν_4	Deg. deform.	71 C		71	

Reference

See No. 62($ZrBr_4$).

No. 67 Hafnium tetraiodide HfI_4
Symmetry T_d **Symmetry number $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	158 B	ia	158	
e	ν_2	Deg. deform.	55 C	ia	55	
f_2	ν_3	Deg. stretch.	224 C		224	
	ν_4	Deg. deform.	63 C		63	

Reference
See No. 62($ZrBr_4$).

No. 68 Osmium tetroxide $Os^{16}O_4$
Symmetry T_d **Symmetry number $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	965 B	ia	965.2	
e	ν_2	Deg. deform.	333 B	ia	333.1	
f_2	ν_3	Deg. stretch.	960 B	960.5	960.1	
	ν_4	Deg. deform.	329 B	329.0	322.7	

References

[1] IR. N. J. Hawkins and W. W. Sabal, J. Chem. Phys. **25**, 775 (1956).
[2] IR. R. E. Dodd, Trans. Faraday Soc. **55**, 1480 (1959).
[3] IR. I. W. Levin and S. Abramowitz, Inorg. Chem. **5**, 2024 (1966).
[4] IR. R. S. McDowell, Inorg. Chem. **6**, 1759 (1967).
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[6] R. C. Davidson, N. Logan, and A. Morris, Chem. Commun. **1968**, 1044.
[7] R. I. W. Levin, Inorg. Chem. **8**, 1018 (1969).
[8] R. J. L. Huston and H. H. Claassen, J. Chem. Phys. **52**, 5646 (1970).
[9] IR. C. G. Barraclough and M. M. Sinclair, Spectrochim. Acta **26A**, 207 (1970).
[10] IR.R. R. S. McDowell and M. Goldblatt, Inorg. Chem. **10**, 625 (1971).

No. 69 Osmium tetroxide $Os^{18}O_4$
Symmetry T_d **Symmetry number $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (CCl_4 soln.)	
a_1	ν_1	Sym. stretch.	910 C	ia	909.7	
e	ν_2	Deg. deform.	317 C	ia	316.6	
f_2	ν_3	Deg. stretch.	912 B	911.8		
	ν_4	Deg. deform.	313 B	312.7		

References

[1] IR. C. G. Barraclough and M. M. Sinclair, Spectrochim. Acta **26A**, 207 (1970).
[2] IR.R. R. S. McDowell and M. Goldblatt, Inorg. Chem. **10**, 625 (1971).

No. 70 Thionitrosyl trifluoride NSF_3

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	NS stretch.	1515 B	1515	1512 p	
	ν_2	NF_3 s-stretch.	775 B	775	768 p	
	ν_3	NF_3 s-deform.	521 B	521	520 dp	
e	ν_4	NF_3 d-stretch.	811 B	811	812 dp	
	ν_5	NF_3 d-deform.	429 B	429	430 dp	
	ν_6	NF_3 rock.	342 B	342	340 dp	

References

[1] IR. H. Richert and O. Glemser, Z. Anorg. Alleg. Chem. **307**, 328 (1961).
[2] R. A. Müller, A. Ruoff, B. Krebs, O. Glemser, and W. Koch, Spectrochim. Acta **25A**, 199 (1969).

No. 71 Trifluorosilane $SiHF_3$

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiH stretch.	2316 B	2315.6 M		
	ν_2	SiF_3 s-stretch.	858 B	858.25 S		
	ν_3	SiF_3 s-deform.	425 B	425.2 M		
e	ν_4	SiF_3 d-stretch.	998 B	997.83 VS		
	ν_5	SiH bend.	844 B	843.6 S		
	ν_6	SiF_3 d-deform.	306 B	306.2 M		

References

[1] IR. C. Newman, S. R. Polo, and M. K. Wilson, Spectrochim. Acta **15**, 793 (1959).
[2] IR. H. Bürger und S. Biedermann, Spectrochim. Acta **27A**, 1687 (1971)

No. 72 Trifluorosilane-d $SiDF_3$

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiD stretch.	1691 B	1690.72		
	ν_2	SiF_3 s-stretch.	854 B	853.84 S		
	ν_3	SiF_3 s-deform.	422 B	422.1 M		
e	ν_4	SiF_3 d-stretch.	992 B	991.76 VS		
	ν_5	SiD bend.	628 B	628.41 M		
	ν_6	SiF_3 d-deform.	303 B	302.8 M		

References

See No. 71($SiHF_3$).

No. 73 Trichlorosilane $SiHCl_3$
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	SiH stretch.	2261 B	2260.9 S	2258 p	
	ν_2	$SiCl_3$ s-stretch.	499 B	498.6 S	489 p	
	ν_3	$SiCl_3$ s-deform.	254 B	253.7 M	250 p	
e	ν_4	SiH bend.	811 B	810.8 VS	799 dp	
	ν_5	$SiCl_3$ d-stretch.	600 B	600.1 VS	587 dp	
	ν_6	$SiCl_3$ d-deform.	176 B	175.5 M	179 dp	

References

[1] R. M. L. Delwaulle and M. F. François, Comptes Rendus **228**, 1007 (1949).
[2] IR.Th. H. Bürger and A. Ruoff, Spectrochim. Acta **26**, 1449 (1970).

No. 74 Trichlorosilane-d $SiDCl_3$
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiD stretch.	1647 B	1647.1 S		
	ν_2	$SiCl_3$ s-stretch.	496 B	495.9 S		
	ν_3	$SiCl_3$ s-deform.	252 B	252.0 M		
e	ν_4	SiD bend.	634 B	633.8 VS		
	ν_5	$SiCl_3$ d-stretch.	550 B	550.0 VS		
	ν_6	$SiCl_3$ d-deform.	175 B	174.5 M		

Reference

[1] IR.Th. H. Bürger and A. Ruoff, Spectrochim. Acta **26**, 1449 (1970).

No. 75 Tribromosilane $SiHBr_3$
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	SiH stretch.	2239 B	2239.2 S	2236 p	
	ν_2	$SiBr_3$ s-stretch.	362 C	362 M, b	362 p	
	ν_3	$SiBr_3$ s-deform.	168 B	168.5 M	166 p	
e	ν_4	SiH bend.	774 C	774 VS	770 dp	
	ν_5	$SiBr_3$ d-stretch.	484 C	483.5 VS	470 dp	
	ν_6	$SiBr_3$ d-deform.	117 C	116.8 W	115 dp	

References

[1] R. M. L. Delwaulle and M. F. François, Comptes Rendus **230**, 743 (1950).
[2] IR.Th. H. Bürger und J. Cichon, Spectrochim. Acta **27A**, 2191 (1971).

No. 76 Phosphoryl fluoride POF_3
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	PO stretch.	1417 B	1415 M	1416.8 p	
	ν_2	PF_3 s-stretch.	873 B	873 M	872.7 p	
	ν_3	PF_3 s-deform.	472 B	473 S	472.4	OV(5) in Raman.
e	ν_4	PF_3 d-stretch.	991 C	990 VS	991.0 dp	
	ν_5	PF_3 d-deform.	482 C	485 M	482.0 dp	
	ν_6	PO bend.	336 C		335.5 dp	

References
[1] R. M. L. Delwaulle and M. F. François, Comptes Rendus **222,** 550 (1946).
[2] IR. H. S. Gutowsky and A. D. Liehr, J. Chem. Phys. **20,** 1652 (1952).
[3] R.Th. R. J. H. Clark and D. M. Rippon, Mol. Phys. **28,** 305 (1974).

No. 77 Phosphoryl chloride $POCl_3$
Symmetry C_2 **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} Gas)	
a_1	ν_1	PO stretch.	1322 C		1321.5	
	ν_2	PCl_3 s-stretch.	481 C		480.5	
	ν_3	PCl_3 s-deform.	266 C		265.5	
e	ν_4	PCl_3 d-stretch.	590 C		589.5	
	ν_5	PO bend.	333 C		332.5	
	ν_6	PCl_3 d-deform.	187 C		187.0	

References
[1] R. M. L. Delwaulle and M. F. François, J. Chim. Physique **45,** 50 (1948).
[2] R.Th. R. J. H. Clark and D. M. Rippon, Mol. Phys. **28,** 305 (1974).

No. 78 Phosphoryl bromide $POBr_3$
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	PO stretch.	1261 D		1261	
	ν_2	PBr_3 s-stretch.	340 D		340	
	ν_3	PBr_3 s-deform.	173 D		173	
e	ν_4	PBr_3 d-stretch.	488 D		488	
	ν_5	PO bend.	267 D		267	
	ν_6	PBr_3 d-deform.	118 D		118	

Reference
See No. 77($POCl_3$).

No. 79 Thiophosphoryl trifluoride PSF_3
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	PF_3 s-stretch.	981 B	981 VS	969 (4.5) p	
	ν_2	PS stretch.	695 B	695 M	696 (100) p	
	ν_3	PF_3 s-deform.	440 B	440 M	441 (20) p	
e	ν_4	PF_3 d-stretch.	945 B	945 VS	937 (6.0) dp	
	ν_5	PF_3 d-deform.	402 C	402 M	404 (13) dp	
	ν_6	PF_3 rock.	275 B	275 W	276 (37) dp	

References

[1] R. M. L. Delwaulle and F. François, Comptes Rendus **226**, 894 (1948).
[2] R. M. L. Delwaulle and F. François, J. Chim. Phys. **46**, 87 (1949).
[3] IR. R. G. Cavell, Spectrochim. Aacta **23A**, 249 (1968).
[4] IR.R. J. R. Durig and J. W. Clark, J. Chem. Phys. **46**, 3057 (1967).

No. 80 Thiophosphoryl trichloride $PSCl_3$
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	PS stretch.	767 B	770	767.2 p	
	ν_2	PCl_3 s-stretch.	432 B	431	431.6 p	
	ν_3	PCl_3 s-deform.	246 C	252	246.0 dp	OV(ν_5).
e	ν_4	PCl_3 d-stretch.	544 C	547	543.7 dp	
	ν_5	PCl_3 d-deform.	246 C	252	246 dp	OV(ν_3).
	ν_6	PCl_3 rock.	167 C	174 (liquid)	167.3 dp	

References

[1] IR. G. Cilento, D. A. Ramsay, and R. N. Jones J. Amer. Chem. Soc. **71**, 2753 (1949).
[2] IR.R. J. R. Durig and J. W. Clark, J. Chem. Phys. **46**, 3057 (1967).
[3] R.Th. R. J. H. Clark and D. M. Rippon, Mol. Phys. **28**, 305 (1974).

No. 81 Perchlorylfluoride $^{35}ClO_3F$
Symmetry C_{3V} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Gas)	
a_1	ν_1	ClO_3 s-stretch.	1063 B	1061 S	1062.5 VS	
	ν_2	ClF stretch.	716 B	714 S	716.0 S	
	ν_3	ClO_3 s-deform.	550 B	549 W	549.5 M	
e	ν_4	ClO_3 d-stretch.	1318 B	1315 VS	1317.5 W	
	ν_5	ClO_3 d-deform.	590 B	590.55 M	589.5 W	
	ν_6	ClO_3 rock.	405 B	405 W	404.5 W	

References
[1] IR. R. P. Madden and W. S. Benedict, J. Chem. Phys. **25**, 594 (1956).
[2] IR. D. R. Lide, Jr. and D. E. Mann, J. Chem. Phys. **25**, 1128 (1956).
[3] R. F. X. Powell and E. R. Lippincott, J. Chem. Phys. **32**, 1883 (1960).
[4] R. H. H. Claassen and E. H. Appleman, Inorg. Chem. **9**, 622 (1970).
[5] R.Th. R. J. H. Clark and D. M. Rippon, Mol. Phys. **28**, 305 (1974).

No. 82 Vanadyl(V) chloride $VOCl_3$
Symmetry C_{3V} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Liquid)	cm⁻¹ (Gas)	
a_1	ν_1	VO stretch.	1042 C	1035 VS	1042.5 (1.8) p	
	ν_2	VCl_3 s-stretch.	408 C	408 S	409.5 (10.0) p	
	ν_3	VCl_3 s-deform.	163 C		163.0 (0.8)	
e	ν_4	VCl_3 d-stretch.	502 C	502 VS	503 (20) dp	
	ν_5	VCl_3 d-deform.	246 C		246.0 (1.5) dp	
	ν_6	VCl_3 rock.	125 C		124.5 (3.8)	

References
[1] R. H. J. Eichoff and F. Weigel, Z. Allg. Chem. **275**, 267 (1954).
[2] IR.R. F. A. Miller and L. R. Cousins, J. Chem. Phys. **26**, 329 (1957).
[3] R. J. R. Beattie, K. M. S. Livingston, D. J. Reynolds, and G. A. Ozin, J. Chem. Soc. **1970**, 1210 (1970).
[4] R.Th. R. J. H. Clark and D. M. Rippon, Mol. Phys. **28**, 305 (1974).

No. 83 Permanganyl fluoride MnO_3F
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	MnO_3 s-stretch.	905 B	905.2 M		
	ν_2	MnF stretch.	721 B	720.7 M		
	ν_3	MnO_3 s-deform.	338 B	337.7 W		
e	ν_4	MnO_3 d-stretch.	953 B	952.5 S		
	ν_5	MnO_3 d-deform.	374 B	373.9 W		
	ν_6	MnF bend.	264 B	264.3 W		

Reference

[1] IR. M. J. Reisfeld, L. B. Asprey, and N. A. Matuiyoff, Spectrochim. Acta **27A**, 765 (1971).

No. 84 Germyl fluoride GeH_3F
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeH_3 s-stretch.	2121 C	2120.6 S		
	ν_2	GeH_3 s-deform.	859 C	859.0 VS		
	ν_3	GeF stretch.	689 B	689.1 S		
e	ν_4	GeH_3 d-stretch.	2132 B	2131.7 S		
	ν_5	GeH_3 d-deform.	874 B	874.0 S		
	ν_6	GeH_3 rock.	643 B	642.6 M		

References

[1] IR. J. E. Griffiths, T. N. Srivastava, and M. Onyszchuk, Can. J. Chem. **40**, 579 (1962).
[2] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).
[3] IR. K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 331 (1965).

No. 85 Germyl fluoride-d_3 GeD_3F
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeD_3 s-stretch.	1525 C	1525		
	ν_2	GeD_3 s-deform.	696 B	696		
	ν_3	GeF stretch.	618 C	618		
e	ν_4	GeD_3 d-stretch.	1535 B	1535		
	ν_5	GeD_3 d-deform.	635 C	635		
	ν_6	GeD_3 rock.	466 C	466		

Reference

[1] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).

No. 86 Germyl chloride GeH_3Cl
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeH_3 s-stretch.	2120 C	2119.9		
	ν_2	GeH_3 s-deform.	848 B	847.5		
	ν_3	GeCl stretch.	422 C	421.7		
e	ν_4	GeH_3 d-stretch.	2129 B	2128.9		
	ν_5	GeH_3 d-deform.	874 B	874.1		
	ν_6	GeH_3 rock.	602 B	602.2		

References
[1] IR. R. C. Lord, Jr., and C. M. Steese, J. Chem. Phys. **22**, 542 (1954).
[2] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).
[3] IR. K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 331 (1965).

No. 87 Germyl chloride-d_3 GeD_3Cl
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				(Gas)		
a_1	ν_1	GeD_3 s-stretch.	1518 C	1518		
	ν_2	GeD_3 s-deform.	609 C	609		
	ν_3	GeCl stretch.	422 C	422		
e	ν_4	GeD_3 d-stretch.	1530 C	1530		
	ν_5	GeD_3 d-deform.	630 C	630		
	ν_6	GeD_3 rock.	434 C	434		

Reference
[1] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).

No. 88 Germyl bromide GeH_3Br
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeH_3 s-stretch.	2115 C	2115.2		
	ν_2	GeH_3 s-deform.	833 C	832.7		
	ν_3	GeBr stretch.	308 C	307.7		
e	ν_4	GeH_3 d-stretch.	2127 B	2126.7		
	ν_5	GeH_3 d-deform.	871 B	870.9		
	ν_6	GeH_3 rock.	578 B	578.2		

References
See No. 84(GeH_3F).

No. 89 Germyl bromide–d$_3$ GeD_3Br
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeD_3 s–stretch.	1514 C	1514		
	ν_2	GeD_3 s–deform.	596 C	596		
	ν_3	GeBr stretch.	305 C	305		
e	ν_4	GeD_3 d–stretch.	1530 C	1530		
	ν_5	GeD_3 d–deform.	621 C	621		
	ν_6	GeD_3 rock.	420 C	420		

Reference

[1] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).

No. 90 Germyl iodide GeH_3I
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeH_3 s–stretch.	2110 C	2110.1		
	ν_2	GeH_3 s–deform.	808 C	808.2		
	ν_3	GeI stretch.	248 C	248.2		
e	ν_4	GeH_3 d–stretch.	2121 B	2120.8		
	ν_5	GeH_3 d–deform.	854 B	853.6		
	ν_6	GeH_3 rock.	558 B	558.3		

References

[1] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).
[2] IR. K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 331 (1965).

No. 91 Germyl iodide–d$_3$ GeD_3I
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeD_3 s–stretch.	1508 C	1508		
	ν_2	GeD_3 s–deform.	582 C	582		
	ν_3	GeI stretch.	249 C	249		
e	ν_4	GeD_3 d–stretch.	1525 C	1525		
	ν_5	GeD_3 d–deform.	603 C	603		
	ν_6	GeD_3 rock.	404 C	404		

Reference

[1] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).

No. 92 Trichlorogermane $GeHCl_3$
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	GeH stretch.	2159 D		2159 p	
	ν_2	$GeCl_3$ s–stretch.	409 D		409 p	
	ν_3	$GeCl_3$ s–deform.	181 D		181 p	
e	ν_4	GeH bend.	699 D		699 dp	
	ν_5	$GeCl_3$ d–stretch.	438 D		438 dp	
	ν_6	$GeCl_3$ d–deform.	149 D		149 dp	

Reference
[1] R. M. L. Delwaulle and M. F. François, Comptes Rendus **228**, **1007 (1949)**.

No. 93 Tribromogermane $GeHBr_3$
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	GeH stretch.	2116 D		2116 p	
	ν_2	$GeBr_3$ s–stretch.	273 D		273 p	
	ν_3	$GeBr_3$ s–deform.	128 D		128 p	
e	ν_4	Ge H bend.	674 D		674 dp	
	ν_5	$GeBr_3$ d–stretch.	325 D		325 dp	
	ν_6	$GeBr_3$ d–deform.	95 E		95 dp	

Reference
[1] R. M. L. Delwaulle and M. F. François, Comptes Rendus **230**, 743 (1950).

No. 94 Rhenium (VII) oxide chloride ReO_3Cl
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	ReO_3 s–stretch.	1001 C	1001.5 VS	1001 S, p	
	ν_2	ReO_3 s–deform.	434 C	434 VS	435 M, p	
	ν_3	ReCl stretch.	293 C	293 S		
e	ν_4	ReO_3 d–stretch.	960 C	960 VS	962.5 M, dp	
	ν_5	ReO_3 d–deform.	344 C	343.5 S	344 M, dp	
	ν_6	ReCl bend.	196 C	196 M	196 S, dp	

References
[1] R. H. J. Eichhoff and F. Weigel, Z. Anorg. Allg. Chem. **275**, 267 (1954).
[2] IR.R. F. A. Miller and G. L. Carlson, Spectrochim. Acta **16**, 1148 (960).
[3] Th. A. Müller, B. Krebs, and W. Höltje, Spectrochim. Acta **23A**, 2753 (1967).

No. 95 Rhenium (VII) oxide bromide ReO_3Br

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (CCl_4 soln.)	cm^{-1}	
a_1	ν_1	ReO_3 s-stretch.	997 C	997 S		
	ν_2	ReO_3 s-deform.	350 C	350 M		
	ν_3	ReBr stretch.	195 C	195 M		
e	ν_4	ReO_3 d-stretch.	963 C	963 VS		
	ν_5	ReO_3 d-deform.	332 C	332 S		
	ν_6	ReBr bend.	168 C	168 M		

References

[1] IR.R. F. A. Miller and G. L. Carlson, Spectrochim. Acta **16,** 1148 (1960).
[2] Th. A. Müller, B. Krebs, and W. Höltje, Spectrochim. Acta **23A,** 2753 (1967).

No. 96 Sulfuryl fluoride SO_2F_2

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1}	
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	SO_2 s-stretch.	1269 C	1269 S	1270 M	
	ν_2	SF_2 s-stretch.	848 C	848 S	847 S	
	ν_3	SO_2 scis.	544 D	544.3 M	543 M	
	ν_4	SF_2 scis.	385 D	384.5 VW		
a_2	ν_5	SF_2 twist.	388 C	ia	388 W	
b_1	ν_6	SO_2 a-stretch.	1502 C	1502 S	1502 VW	
	ν_7	SO_2 rock.	553 D	552.8 M		
	ν_8	SF_2 a-stretch.	885 C	885 S	883 VW	
	ν_9	SO_2 wag.	539 D	539.4 M		

References

[1] IR. W. D. Perkins and M. K. Wilson, J. Chem. Phys. **20,** 1791 (1952).
[2] R. P. Bender and J. M. Wood, Jr., J. Chem. Phys. **23,** 1316 (1955).
[3] Th. G. R. Hunt and M. K. Wilson, Spectrochim. Acta **18,** 959 (1962).
[4] IR. D. R. Lide, Jr., D. E. Mann, and J. J. Comeford, Spectrochim. Acta **21,** 497 (1965).
[5] Th. H. Toyuki and K. Shimizu, Bull. Chem. Soc. Japan, **39,** 2364 (1966).
[6] IR. A. J. Sumodi and E. L. Pace, Spectrochim. Acta **28A,** 1129 (1972).

No. 97 Sulfuryl chloride SO_2Cl_2
Symmetry C_{2V} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Lquid)	
a_1	ν_1	SO_2 s–stretch.	1205 C	1205 S	1182 S, p	
	ν_2	SO_2 scis.	577 D	577 VS	560 VS, p	
	ν_3	SCl_2 s–stretch.	408 D		408 VS, p	
	ν_4	SCl_2 scis.	218 D		218 VS, p	
a_2	ν_5	SO_2 twist.	282 D	ia	282 S, dp	
b_1	ν_6	SO_2 a–stretch.	1434 C	1434 S	1414 M, dp	
	ν_7	SO_2 rock.	388 D		388 S, dp	
b_2	ν_8	SCl_2 a–stretch.	586 D	586 VS	580 VW, dp	
	ν_9	SO_2 wag.	362 D		362 sh, dp	

References
[1] R. R. Vogel–Hogler, Acta. Phys. Austriaca, **1**, 323 (1948).
[2] IR. D. E. Martz and R. T. Lagemann, J. Chem. Phys. **22**, 1193 (1954).
[3] R. R. J. Gillespie and E. A. Robinson, Can. J. Chem. Phys. **39**, 2171 (1961).
[4] Th. G. R. Hunt and M. K. Wilson, Spectrochim. Acta **18**, 959 (1962).
[5] Th. H. Toyuki and K. Shimizu, Bull. Chem. Soc. Japan **39**, 2364 (1966).

No. 98 Dichlorosilane SiH_2Cl_2
Symmetry C_{2V} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	SiH_2 s–stretch.	2224 C	2224 S	2221 S, p	
	ν_2	SiH_2 scis.	954 C	954 S	942 W, dp	
	ν_3	$SiCl_2$ s–stretch.	527 C	527 W	514 S, p	
	ν_4	$SiCl_2$ scis.	188 D		188 M, dp	
a_2	ν_5	SiH_2 twist.	710 D	ia	710 W, dp	
b_1	ν_6	SiH_2 a–stretch.	2237 B	2237 S		
	ν_7	SiH_2 rock.	602 C	602 W		
b_2	ν_8	SiH_2 wag.	876 B	876 VS	868 VW, dp	
	ν_9	$SiCl_2$ a–stretch.	590 C	590 S	566 VW, dp	

References
[1] IR.R. J. A. Hawkins and M. K. Wilson, J. Chem. Phys. **21**, 360 (1953).
[2] IR. J. A. Hawkins, S. R. Polo, and M. K. Wilson, J. Chem. Phys. **21**, 1122 (1953).
[3] IR. D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **27**, 489 (1968).
[4] Th. D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **33**, 425 (1970).

No. 99 Dichlorosilane-d_2 SiD_2Cl_2
Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiD_2 s-stretch.	1608 C	1608 S		
	ν_2	SiD_2 scis.	695 C	695 S		
	ν_3	$SiCl_2$ s-stretch.	519 C	519 W		
	ν_4	$SiCl_2$ scis.	187 D	187 W		
a_2	ν_5	SiD_2 twist.	506 D	ia		CF.
b_1	ν_6	SiD_2 a-stretch.	1637 C	1637 S		
	ν_7	SiD_2 rock.	466 B	466 W		
b_2	ν_8	SiD_2 wag.	663 B	663 VS		
	ν_9	$SiCl_2$ a-stretch.	566 C	566 W		

References

[1] IR. D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **27**, 489 (1968).
[2] Th. D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **33**, 425 (1970).

No. 100 Dibromosilane SiH_2Br_2
Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	SiH_2 s-stretch.	2206 D	2200 S	2206 S, p	
	ν_2	SiH_2 scis.	942 C	942 VS	925 W, dp	
	ν_3	$SiBr_2$ s-stretch.	407 C	407 M	393 S, p	
	ν_4	$SiBr_2$ scis.	122 D		122 M, p	
a_2	ν_5	SiH_2 twist.	688 D	ia	688 W, dp	
b_1	ν_6	SiH_2 a-stretch.	2232 D	2200 S	2232 W, dp	
	ν_7	SiH_2 rock.	556 C	556 S		
b_2	ν_8	SiH_2 wag.	843 C	843 VS	828 VW, dp	
	ν_9	$SiBr_2$ a-stretch.	471 C	471 S	456 W, dp	

References

[1] R. F. François and M. Buisset, Comptes Rendus **230**, 1946 (1950).
[2] IR. D. W. Mayo, H. E. Opitz, and J. S. Peake, J. Chem. Phys. **23**, 1344 (1955).

No. 101 Selenium dioxide difluoride SeO_2F_2
Symmetry C_{2V} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	SeO_2 s-stretch.	973 C	973 S	969 S, p	
	ν_2	SeF_2 s-stretch.	700 C	700 S	702 S, p	
	ν_3	SeO_2 scis.	360 C	360 S	357 M	
	ν_4	SeF_2 scis.	284 C	284 W	280 M	
a_2	ν_5	SeF_2 twist.	272 E			OV($2\nu_5$).
b_1	ν_6	SeO_2 a-stretch.	1059 C	1059 S	1059 W	
	ν_7	SeO_2 rock.	335 D	335 S	334 M	OV(ν_9).
b_2	ν_8	SeF_2 s-stretch.	756 C	756 W		
	ν_9	SeO_2 wag.	335 D	335 S	334 M	OV(ν_7).

References

[1] R. R. Paetzold and K. H. Ziegenbalg, Z. Chem. **4**, 461 (1964).
[2] IR.R. T. Birchall and R. J. Gillespie, Spectrochim. Acta **22**, 681 (1966).

No. 102 Nitric acid $H^{14}NO_3$
Symmetry C_S Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OH stretch.	3550 B	3550.0 M		
	ν_2	NO_2 a-stretch.	1708 B	1708.2 VS		
	ν_3	OH bend.	1331 B	1330.7 S		
	ν_4	NO_2 s-stretch.	1325 B	1324.9 VS		
	ν_5	NO_2 scis.	879 B	878.6 S		
	ν_6	NO stretch.	647 B	646.6 W		
	ν_7	NO_2 rock.	579 B	579.0 W		
a''	ν_8	NO_2 wag.	762 B	762.2 S		
	ν_9	Torsion	456 B	455.8 M		

Reference

[1] IR. G. E. McGraw, D. L. Bernitt, and I. C. Hisatsune, J. Chem. Phys. **42**, 237 (1965).

No. 103 Nitric acid-d $D^{14}NO_3$
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OD stretch.	2622 B	2621.5 M		
	ν_2	NO_2 a-stretch.	1687 B	1687.0 VS		
	ν_3	NO_2 s-stretch.	1308 B	1308.4 VS		
	ν_4	OD bend.	1014 B	1013.6 M		
	ν_5	NO_2 scis.	888 B	888.0 S		
	ν_6	NO stretch.	641 B	641.0 S		
	ν_7	NO_2 rock.	541 B	541.0 W		
a''	ν_8	NO_2 wag.	763 B	762.8 S		
	ν_9	Torsion	342 B	342.0 M		

Reference

See No. 102($H^{14}NO_3$).

No. 104 Nitric acid $H^{15}NO_3$
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OH stretch.	3550 B	3550.0 M		
	ν_2	NO_2 a-stretch.	1672 B	1672.0 VS		
	ν_3	OH bend.	1327 B	1327.0 S		
	ν_4	NO_2 s-stretch.	1321 B	1320.6 S		
	ν_5	NO_2 scis.	871 B	870.8 S		
	ν_6	NO stretch.	647 B	646.6 W		
	ν_7	NO_2 rock.	578 B	578.0 W		
a''	ν_8	NO_2 wag.	744 B	743.6 S		
	ν_9	Torsion	456 B	455.9 M		

Reference

See No. 102($H^{14}NO_3$).

No. 105 Nitric acid–d $D^{15}NO_3$
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				(Gas)		
			cm^{-1}	cm^{-1}	cm^{-1}	
a'	ν_1	OD stretch.	2622 B	2621.9 M		
	ν_2	NO_2 a–stretch.	1656 B	1655.5 VS		
	ν_3	NO_2 s–stretch.	1291 B	1290.7 S		
	ν_4	OD bend.	1012 B	1011.5 M		
	ν_5	NO_2 scis.	876 B	876.3 S		
	ν_6	NO stretch.	641 B	640.9 S		
	ν_7	NO_2 rock.	541 B	541.0 VW		
a''	ν_8	NO_2 wag.	743 B	743.4 S		
	ν_9	Torsion	345 D			OV($\nu_7+\nu_9$, $\nu_8+\nu_9$).

Reference

See No. 102($H^{14}NO_3$).

No. 106 Fluoronitrate $FO^{14}NO_2$
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO_2 a–stretch.	1759 C	1759.1 VS		
	ν_2	NO_2 s–stretch.	1301 B	1300.9 VS		
	ν_3	OF stretch.	928 B	927.7 S		
	ν_4	NO_2 scis.	804 B	803.7 S		
	ν_5	NO stretch.	633 B	633.0 VW		
	ν_6	NO_2 rock.	455 B	454.5 MS		
	ν_7	OF bend.	303 B	302.6 VW		
a''	ν_8	NO_2 wag.	709 C	708.5 M		
	ν_9	OF torsion	152 B	151.6 VVW		

References

[2] IR. A. J. Arvia, L. F. R. Cafferata, and H. J. Schumacher, Chem. Ber. **96,** 1187 (1963).
[2] IR. R. H. Miller, P. L. Bernitt, and I. C. Hisatsune, Spectrochim. Acta **23A,** 223 (1967).

No. 107 Fluoronitrate $FO^{15}NO_2$
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO a–stretch.	1720 C	1719.8 VS		
	ν_2	NO_2 s–stretch.	1291 B	1290.5 VS		
	ν_3	OF stretch.	928 B	927.5 S		
	ν_4	NO_2scis.	792 B	791.8 S		
	ν_5	NO stretch.	632 B	631.5 VW		
	ν_6	NO_2 rock.	455 B	454.4 MS		
	ν_7	OF bend.	302 B	301.6 VW		
a''	ν_8	NO_2 wag.	690 C	690.2 M		
	ν_9	OF torsion	151 D	151.2		OC($\nu_1+\nu_9$, $\nu_1-\nu_9$, $\nu_3+\nu_9$).

References

See No. 106($FO^{14}NO_2$).

No. 108 Chloronitrate $ClO^{14}NO_2$
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO_2 a–stretch.	1735 B	1735.4 VS		
	ν_2	NO_2 s–stretch.	1292 B	1291.9 VS		
	ν_3	OCl stretch.	809 C	809.3 S		
	ν_4	NO_2 scis.	780 C	780.2 MS		
	ν_5	NO stretch.	560 B	560.0 S		
	ν_6	NO_2 rock.	434 B	434.1 M		
	ν_7	OCl bend.	270 C	270 VVW		
a''	ν_8	NO_2 wag.	711 B	710.8 W		
	ν_9	OCl torsion	121 E	121		OC($\nu_5+\nu_7-\nu_9$).

References

[1] IR. K. Brandle, M. Schmeisser, and W. Luttke, Chem. Ber. **93**, 2300 (1960).
[2] IR. A. J. Arvia, L. F. R. Cafferata, and H. J. Schumacher, Chem. Ber. **96**, 1187 (1963).
[3] IR. R. H. Miller, P. L. Bernitt, and I. C. Hisatsune, Spectrochim. Acta **23A**, 223 (1967).

No. 109 Chloronitrate $ClO^{15}NO_2$
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NO_2 a–stretch.	1694 B	1694.0 VS		
	ν_2	NO_2 s–stretch.	1280 B	1280.2 VS		
	ν_3	OCl stretch.	805 C	804.7 MS		
	ν_4	NO_2 scis.	773 C	772.9 S		
	ν_5	NO stretch.	557 B	556.8 S		
	ν_6	NO_2 rock.	432 B	432.2 M		
	ν_7	OCl bend.	263 D	263		OC($\nu_5+\nu_7$).
a''	ν_8	NO_2 wag.	694 B	693.7 W		
	ν_9	OCl torsion	122 E	122		OC($\nu_5+\nu_7-\nu_9$).

References

[1] IR. K. Brandle, M. Schmeisser, and W. Luttke, Chem. Ber. **93**, 2300 (1960).
[2] IR. A. J. Arvia, L. F. R. Cafferata, and H. J. Schumacher, Chem. Ber. **96**, 1187 (1963).
[3] IR. R. H. Miller, P. L. Bernitt, and I. C. Hisatsune, Spectrochim. Acta **23A**, 223 (1967).

No. 110 Phosphoryl dichlorofluoride $POCl_2F$
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Liquid)	
a'	ν_1	PO stretch.	1331 D		1331 p	
	ν_2	PF stretch.	894 D		894 p	
	ν_3	PCl_2 s–stretch.	547 D		547 p	
	ν_4	PO ip–bend.	386 D		386 p	
	ν_5	PF bend.	330 D		330 p	
	ν_6	PCl_2 scis.	207 D		207 p	
a''	ν_7	PCl_2 a–stretch.	620 D		620 dp	
	ν_8	PO op–bend.	372 D		372 dp	
	ν_9	PCl_2 rock.	254 D		254 dp	

Reference

[1] R. M. L. Delwaulle and F. François, Comptes Rendus **222**, 550 (1946).

No. 111 Phosphoryl dibromofluoride $POBr_2F$

Symmetry C_S Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Liquid)	
a'	ν_1	PO stretch.	1303 D		1303 p	
	ν_2	PF stretch.	880 D		880 p	
	ν_3	PBr_2 s–stretch.	466 D		466 p	
	ν_4	PO ip–bend.	306 D		306 p	
	ν_5	PF bend.	273 D		273 p	
	ν_6	PBr_2 scis.	134 D		134 p	
a''	ν_7	PBr_2 a–stretch.	538 D		538 dp	
	ν_8	PO op–bend.	291 D		291 dp	
	ν_9	PBr_2 rock.	220 D		220 dp	

Reference

See No. 110($POCl_2F$).

No. 112 Thiophosphoryl chlorodifluoride $PSClF_2$

Symmetry C_S Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	PF_2 s–stretch.	946 B	946 VS	939 (3.7) p	
	ν_2	PS stretch.	738 B	738 VS	727 (50) p	
	ν_3	PCl stretch.	541 B	541 S	536 (100) p	
	ν_4	PCl bend.	395 B	395 M	394 (31) p	
	ν_5	PF_2 scis.	361 B	361 M	359 (38) p	
	ν_6	PS ip–bend.	207 C	198	207 (65) p	
a''	ν_7	PF_2 s–stretch.	920 B	920 VS	913 (6.5) dp	
	ν_8	PF_2 rock.	317 B	317 M	314 (14) dp	
	ν_9	PS op–bend.	251 C		251 (14) dp	

Reference

[1] IR.R. J. R. Durig and J. W. Clark, J. Chem. Phys. **46**, 3057 (1967).

No. 113 Thiophosphoryl dichlorofluoride $PSCl_2F$

Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	PF stretch.	912 B	912 VS	902 (2) p	
	ν_2	PS stretch.	753 B	753 VS	737 (17) p	
	ν_3	PCl_2 s-stretch.	478 B	478 S	474 (100) p	
	ν_4	PF bend.	331 B	331 M	327 (13) dp	
	ν_5	PS ip-bend.	268 B	268 M	267 (32) p	
	ν_6	PCl_2 scis.	192 D	192 W	193 (65) dp	OV(ν_9).
a''	ν_7	PCl_2 a-stretch.	575 C	575 S	567 (6) dp	
	ν_8	PS op-bend.	319 B	319 M	317 (19) dp	
	ν_9	PCl_2 rock.	192 D	192 W	193 (65) dp	OV(ν_6).

Reference

See No. 112($PSClF_2$).

No. 114 Phosphorus pentafluoride PF_5

Symmetry D_{3h} **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	PF_3 s-stretch.	816 B		816 (10) p	
	ν_2	PF_2 s-stretch.	648 C		648 (1b) p	
a_2''	ν_3	PF_2 a-stretch.	947 B	946.6 VS		
	ν_4	PF_3 op-deform.	575 B	575.1 M		
e'	ν_5	PF_3 d-stretch.	1024 B	1024 VS	1029 (1b)	
	ν_6	PF_3 d-deform.	533 B	532.5 M	535 (1sh) dp	
	ν_7	PF bend.	174 C		174 (1b) dp	
e''	ν_8	PF bend.	520 C		520 (1b) dp	

References

[1] IR. J. E. Griffiths, R. P. Carter, and R. R. Holmes, J. Chem. Phys. **41**, 863 (1964).
[2] IR. L. C. Hoskins, J. Chem. Phys. **42**, 2631 (1965).
[3] IR. J. E. Griffiths, J. Chem. Phys. **42**, 2632 (1965).
[4] IR.R. L. C. Hoskins and R. C. Lord, J. Chem. Phys. **46**, 2402 (1967).
[5] IR. R. M. Deiters and R. R. Holmes, J. Chem. Phys. **48**, 4796 (1968).
[6] R. I. W. Levin, J. Chem. Phys. **50**, 1031 (1969).
[7] Th. I. W. Levin, J. Mol. Spectry. **33**, 61 (1970).
[8] R. F. A. Miller and R. J. Capwell, Spectrochim. Acta **27A**, 125 (1971).

No. 115 Phosphorus trichloride difluoride PCl_3F_2

Symmetry D_{3h} Symmetry number $\sigma = 6$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	PF_2 s-stretch.	633 C		633 M, p	
	ν_2	PCl_3 s-stretch.	387 C		387 S, p	
a_2''	ν_3	PF_2 a-stretch.	867 C	867 VS		
	ν_4	PCl_3 op-deform.	328 C	328 M		
e'	ν_5	PCl_3 d-stretch.	625 C	625 VS	609 VW, dp	
	ν_6	PCl_3 d-deform.	404 C	404 VS	408 M, dp	
	ν_7	PF bend.	122 C		122 S, dp	
e''	ν_8	PF bend.	357 C		357 W, dp	

References

[1] IR.R. J. E. Griffiths, R. P. Carter, Jr., and R. R. Holmes, J. Chem. Phys. **41**, 863 (1964).
[2] Th. R. R. Holmes, R. M. Deiters, and J. A. Golen, Inorg. Chem. **8**, 2612 (1969).
[3] Th. I. R. Beattie, K. M. S. Livingston, and D. J. Reynolds, J. Chem. Phys. **51**, 4269 (1969).

No. 116 Phosphorus pentachloride PCl_5

Symmetry D_{3h} Symmetry number $\sigma = 6$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (C_6H_6 or CS_2 soln.)	
a_1'	ν_1	PCl_3 s-stretch.	395 D		395 VS, p	
	ν_2	PCl_2 s-stretch.	370 D		370 VW	
a_2''	ν_3	PCl_2 a-stretch.	465 C	465 VS	441 VW	
	ν_4	PCl_3 op-deform.	299 D	299 S (CS_2 soln.)	301	
e'	ν_5	PCl_3 d-stretch.	592 C	592 VS	581 W, p	
	ν_6	PCl_3 d-deform.	273 D	273 S (CS_2 soln.)	281 W, dp	
	ν_7	PCl bend.	100 C	100 W	100 M, dp	
e''	ν_8	PCl bend.	261 D		261 W, dp	

References

[1] R. H. Moureu, P. Sue, and M. Magat, Contribution a l· étude de la structure moleculaire. Vol. commem. Victor Herni, p.125 Maison Desoerg, Liege (1947/48).
[2] IR.R. J. K. Wilmshurst and H. J. Bernstein, J. Chem. Phys. **27**, 661 (1957).
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[4] R. M. J. Taylor and L. A. Woodward, J. Chem. Soc. **1963**, 4670 (1963).
[5] Th. R. R. Holmes, R. M. Deiters, and J. A. Golen, Inorg. Chem. **8**, 2612 (1969).
[6] Th. R. R. Holmes and R. M. Deiters, J. Chem. Phys. **51**, 4043 (1969).

No. 117 Vanadium pentafluoride VF_5
Symmetry D_{3h} **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	VF_3 s-stretch.	718 B		718 VS	
	ν_2	VF_2 s-stretch.	608 B		608 M	
a_2''	ν_3	VF_2 a-stretch.	784 B	784 S		
	ν_4	VF_3 op-deform.	331 B	331 W		
e'	ν_5	VF_3 d-stretch.	810 C	810 M	812 W	
	ν_6	VF_3 d-deform.	282 C	282 M	286 VW	
	ν_7	VF bend.	110 D	109.5 M	99 W	
e''	ν_8	VF bend.	336 B		336 M	

References
[1] IR. R. G. Cavell and H. C. Clark, Inorg. Chem. **3**, 1789 (1964).
[2] IR.R. H. H. Claassen and H. Selig, J. Chem. Phys. **44**, 4039 (1966).
[3] IR.R. I. R. Beattie, K. M. S. Livingston, G. A. Ozin, and D. J. Reynolds, J. Chem. Soc. A**1969**, 958.
[4] IR.R. H. Selig, J. H. Holloway, J. Tyson, and H. H. Claassen, J. Chem. Phys. **53**, 2559 (1970).

No. 118 Arsenic pentafluoride AsF_5
Symmetry D_{3h} **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	AsF_3 s-stretch.	734 C		734.3 VS, p	
	ν_2	AsF_2 s-stretch.	644 C		644 M, p?	
a_2''	ν_3	AsF_2 a-stretch.	787 B	787.4 VS		
	ν_4	AsF_3 op-deform.	400 B	400.4 S		
e'	ν_5	AsF_3 d-stretch.	811 B	811.4 VS	813 M, dp	
	ν_6	AsF_3 d-deform.	372 C	372 S	366	
					(Liquid)	
	ν_7	AsF bend.	123 C	123 W	130 M, dp	
e''	ν_8	AsF bend.	386 C		386 M, dp	

References
[1] IR.R. L. C. Hoskins and R. C. Lord, J. Chem. Phys. **46**, 2402 (1967).
[2] Th. I. W. Levin, J. Mol. Spectry. **33**, 61 (1970).
[3] R. H. Selig, J. H. Holloway, J. Tyson, and H. H. Claassen, J. Chem. Phys. **53**, 2559 (1970).
[4] IR. L. C. Hoskins and C. N. Perng, J. Chem. Phys. **55**, 5063 (1971).

No. 119 Antimony pentachloride $SbCl_5$

Symmetry D_{3h} Symmetry number $\sigma = 6$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	$SbCl_3$ s-stretch.	357 C		357 (10) p	
	ν_2	$SbCl_2$ s-stretch.	307 C	306 W (liquid)	307 (4) dp	
a_2''	ν_3	$SbCl_2$ a-stretch.	384 C	384 VS		
	ν_4	$SbCl_3$ op-deform.	154 D	154 (CCl_4 soln.)		
e'	ν_5	$SbCl_3$ d-stretch.	398 C	398 VS	397 (2)	
	ν_6	$SbCl_3$ d-deform.	177 C	172 S (CCl_4 soln.)	177 (4) dp	
	ν_7	SbCl bend.	72 D		72 dp	
e''	ν_8	SbCl bend.	165 C		165 (2) dp	

References

[1] IR. J. K. Wilmshurst, J. Mol. Spectry. **5**, 343 (1960).
[2] IR.R. G. L. Carlson, Spectrochim. Acta **19**, 1291 (1963).
[3] Th. R. R. Holmes, R. M. Deiters, and J. A. Golen, Inorg. Chem. **8**, 2612 (1969).
[4] Th. R. R. Holmes and R. M. Deiters, J. Chem. Phys. **51**, 4043 (1969).

No. 120 Tellurium hexafluoride TeF_6

Symmetry O_h Symmetry number $\sigma = 24$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{2g}	ν_1	Sym. stretch.	697 B	ia	697.1 VS	
e_g	ν_2	Deg. stretch.	670 C	ia	670.3 W	
f_{1u}	ν_3	Deg. stretch.	751 C	751.0	ia	
	ν_4	Deg. deform.	327 C	326.5	ia	
f_{2g}	ν_5	Deg. deform.	314 C	ia	314 W	
f_{2u}	ν_6	Deg. deform.	197 E	ia	ia	OC($2\nu_6$) [3].

References

[1] IR.R. B. Weinstock and Goodman, Advan. Chem. Phys. **9**, 169 (966), and references cited there.
[2] IR. S. Abramowitz and I. W. Levin, J. Chem. Phys. **44**, 3353 (1966).
[3] R. H. H. Claassen, G. L. Goodman, J. H. Holloway, and H. Selig, J. Chem. Phys. **53**, 341 (1970).

No. 121 Iridium(VI)fluoride IrF_6
Symmetry O_h **Symmetry number $\sigma = 24$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	Sym. stretch.	702 B	ia	701.7 VS, p	
e_g	ν_2	Deg. stretch.	645 C	ia	645 W, dp	
f_{1u}	ν_3	Deg. stretch.	720 B	719.8 S	ia	
	ν_4	Deg. deform.	276 B	276.0 S	ia	
f_{2g}	ν_5	Deg. deform.	267 C	ia	267 W, dp	
f_{2u}	ν_6	Deg. deform.	206 D	ia	ia	OC($\nu_2+\nu_6$, $\nu_2-\nu_6$, $\nu_5+\nu_6$). [1].

References

[1] IR.R. B. Weinstock and G. L. Goodman, Advan. Chem. Phys. **9**, 169 (1966), and references cited there.
[2] R. H. H. Claassen and H. Selig, Israel J. Chem. **7**, 449 (1969).
[3] IR. H. Kim, P. A. Souder, and H. H. Claassen, J. Mol. Spectry. **26**, 46 (1968).

No. 122 Sulfur chloride pentafluoride $SClF_5$
Symmetry C_{4v} **Symmetry number $\sigma = 4$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	SF stretch.	855 B	854.6 VS	833 W, p	
	ν_2	SF_4 s-stretch.	707 B	707.2 VS	704 S, p	
	ν_3	SF_4 op-deform.	602 B	601.9 VS	603 W, p	
	ν_4	SCl stretch.	402 B	401.7 VS	403 VS, p	
b_1	ν_5	SF_4 a-stretch.	625 C	ia	625 M, dp	
	ν_6	SF_4 op-deform.	271 C	ia	271 M, dp	
b_2	ν_7	SF_4 ip-deform.	505 C	ia	505 W, dp	
e	ν_8	SF_4 d-stretch.	909 B	909.0 VS	927 W, dp	
	ν_9	SF bend.	579 B	579.0 M	584 VW, dp	
	ν_{10}	SF_4 ip-deform.	441 B	441.0 S	442 M, dp	
	ν_{11}	SCl bend.	397 B	396.5 S	396 S, dp	

References

[1] IR.R. L. H. Cross, H. L. Roberts, P. Goggin, and L. A. Woodward, Trans. Faraday Soc. **56**, 945 (1960).
[2] IR.R. J. E. Griffiths, Spectrochim. Acta **23A**, 2145 (1967).

No. 123 Tungsten chloride pentafluoride $WClF_5$

Symmetry C_{4v} Symmetry number $\sigma = 4$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a_1	ν_1	WF stretch.	743 C	743 M	744 VS, p	
	ν_2	WF_4 s-stretch.	703 C	703 VS	703 M, p	
	ν_3	WCl stretch.	400 C	400 VS	407 S, p	
	ν_4	WF_4 op-deform.	254 C	254 VS	257 W	
b_1	ν_5	WF_4 a-stretch.	644 D	ia	644 W	
	ν_6	WF_4 op-deform.	182 D	ia	182 W	
b_2	ν_7	WF_4 ip-deform.	377 D	ia	377 M, dp	
e	ν_8	WF_4 d-stretch.	671 C	671 S	661 M, dp	
	ν_9	WF bend.	302 C	302 M	307 M, dp	
	ν_{10}	WF_4 ip-deform.	278 C	278 S	290 W	
	ν_{11}	WCl bend.	228 C	228 S	227 W	

Reference

[1] IR.R. D. M. Adams, G. W. Fraser, D. M. Morris, and R. D. Peacock, J. Chem. Soc. **A 1968,** 1131.

No. 124 Iodine heptafluoride IF_7

Symmetry D_{5h} Symmetry number $\sigma = 10$

Sym. class	No.	Approximate type of mode[a]	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Gas)	
a_1'	ν_1	IF_{ax} s-stretch.	676 C	ia	676 W, p	
	ν_2	IF_{eq} s-stretch.	635 C	ia	635 S, p	
a_2''	ν_3	IF_{ax} a-stretch.	672 C	672 VS	ia	
	ν_4	$F_{eq}IF_{ax}$ deform.	257 C	257 W	ia	
e_1'	ν_5	IF_{eq} a-stretch.	746 C	746 S, b	ia	
	ν_6	$F_{eq}IF_{eq}$ deform.	425 C	425 VS	ia	
	ν_7	$F_{ax}IF_{ax}$ deform.	363 C	363 S	ia	
e_1''	ν_8	$F_{eq}IF_{ax}$ deform.	310 C	ia	310 W, dp	
e_2'	ν_9	IF_{eq} a-stretch.	510 C	ia	510 W, dp	
	ν_{10}	$F_{eq}IF_{eq}$ deform.	352 C	ia	352 W, dp	
e_2''	ν_{11}	$F_{eq}IF_{ax}$ deform.	200 D	ia	ia	CF[2]. OC($\nu_2+\nu_{11}$, $\nu_5+\nu_{11}$).

[a] F_{ax} and F_{eq} represent the axial and equatorial fluorine atoms, respectively.

References

[1] IR.R. H. H. Claassen, E. L. Gasner, and H. Salig, J. Chem. Phys. **49,** 1803 (1968).
[2] IR.R.Th. H. H. Eysel and K. Seppelt, J. Chem. Phys. **56,** 5081 (1972).
[3] Th. E. Wendling and S. Rahmondi, Bull. Soc. Chim. (France) **1,** 33 (1972).

No. 125 Digermane GeH_3GeH_3
Symmetry D_{3d} **Symmetry number σ = 6**

-sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_{1g}	ν_1	GeH_3 s-stretch.	2068 C	ia	2068 S, p	
	ν_2	GeH_3 s-deform.	832 C	ia	832 VW, p	
	ν_3	GeGe stretch.	268 C	ia	268.4 S, p	
a_{1u}	ν_4	Torsion	146 E[a]	ia	ia	
a_{2u}	ν_5	GeH_3 s-stretch.	2077 B	2077.0 VS	ia	
	ν_6	GeH_3 s-deform.	756 B	756.0 VS	ia	
e_u	ν_7	GeH_3 d-stretch.	2091 B	2090.7 S	ia	
	ν_8	GeH_3 d-deform.	879 B	879.0 S	ia	
	ν_9	GeH_3 rock.	370 B	370.3 M	ia	
e_g	ν_{10}	GeH_3 d-stretch.	2081 E	ia		CF[4].
	ν_{11}	GeH_3 d-deform.	880 C	ia	879.6 M, dp	
	ν_{12}	GeH_3 rock.	567 C	ia	566.6 W, dp	

[a] Estimated from combination bands.

References

[1] IR. D. A. Dows and R. M. Hexter, J. Chem. Phys. **24**, 1029 (1956).
[2] IR.R. V. A. Crawford, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **37**, 2377 (1962).
[3] IR.R. J. E. Griffiths and G. E. Walraffen, J. Chem. Phys. **40**, 321 (1964).
[4] Th. E. A. Clark and A. Weber, J. Chem. Phys. 45, 1759 (1966).

No. 126 Digermane-d_6 GeD_3GeD_3
Symmetry D_{3d} **Symmetry number σ = 6**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_{1g}	ν_1	GeD_3 s-stretch.	1484 C	ia	1483.7 S, p	
	ν_2	GeD_3 s-deform.	600 C	ia	600 VW, p	
	ν_3	GeGe stretch.	264 C	ia	264 S, p	CF[3].
a_{1u}	ν_4	Torsion	106 E[a]	ia	ia	
a_{2u}	ν_5	GeD_3 s-stretch.	1490 B	1489.9 VS	ia	
	ν_6	GeD_3 s-deform.	546 C	546.2 S	ia	
	ν_8	GeD_3 d-deform.	630 B	629.7 M	ia	
e_u	ν_7	GeD_3 d-stretch.	1511 C	1511 S	ia	
	ν_9	GeD_3 rock.	262 C	262 S	ia	
e_g	ν_{10}	GeD_3 d-stretch.	1501 D	ia	1501	
	ν_{11}	GeD_3 d-deform.	626 C	ia	626.1 M, dp	
	ν_{12}	GeD_3 rock.	412 C	ia	412.0 W, dp	

[a] From the product rule.

References

[1] IR.R. V. A. Crawford, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **37**, 2377 (1962).
[2] IR.R. J. E. Griffiths and G. E. Walraffen, J. Chem. Phys. **40**, 321 (1964).
[3] Th. E. A. Clark and A. Weber, J. Chem. Phys. 45, 1759 (1966).

No. 127 Cyanogen fluoride FCN
Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	CN stretch.	2323 C	2323		
π	ν_2	Deform.	451 A	451.32		
σ^+	ν_3	CF stretch.	1077 A	1076.52		

References
[1] IR. R. E. Dodd and R. Little, Spectrochim. Acta **16,** 1083 (1960).
[2] IR. A. R. H. Cole, L. Isaacson, and R. C. Lord, Spectrochim. Acta **23,** 86 (1967).
[3] Th. A. Ruoff, Spectrochim. Acta **26A,** 545 (1970).

No. 128 Cyanogen iodide ICN
Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	CN stretch.	2188 C	2188.0		
π	ν_2	Deform.	305 C	304.5		
σ^+	ν_3	CI stretch.	486 C	485.8		

References
[1] IR. S. Hemple and E. R. Nixon, J. Chem. Phys. **47,** 4273 (1967).
[2] Th. A. Ruoff, Spectrochim. Acta **26A,** 545 (1970).

No. 129 Carbonyl fluoride COF_2
Symmetry C_{2v} **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CO stretch.	1928 C	1928 VS	1944 VW	
	ν_2	CF_2 s-stretch.	965 B	965 VS	965 VS	
	ν_3	CF_2 deform.	584 C	584 M	571 W	
b_1	ν_4	CF_2 a-stretch.	1249 B	1249 VS	1238 VW	
	ν_5	CO deform.	626 C	626 M	620 M	
b_2	ν_6	Op-deform.	774 B	774 M	771 VW	

References
[1] IR.R. A. H. Nielsen, T. G. Burke, P. J. H. Woltz, and E. A. Jones, J. Chem. Phys. **20,** 596 (1952).
[2] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32,** 1296 (1960).

No. 130 Carbonyl chloride $COCl_2$
Symmetry C_{2V} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a_1	ν_1	CO stretch.	1827 B	1827 VS	1807 M	
	ν_2	CCl_2 s-stretch.	567 C	567 M	573 VS	
	ν_3	CCl_2 deform.	285 C	285 W	302 S	
b_1	ν_4	CCl_2 a-stretch.	849 B	849 S	832 VW	
	ν_5	CO deform.	440 C	440 M	442 M	
b_2	ν_6	Op-deform.	580 C	580 M		

References

[1] IR.R. A. H. Nielsen, T. G. Burke, P. J. H. Woltz, and E. A. Jones, J. Chem. Phys. **20**, 596 (1952).
[2] IR. E. Catalano and K. S. Pitzer, J. Amer. Chem. Soc. **80**, 1054 (1958).
[3] IR.R. J. Overend and J. C. Evans, Trans. Faraday Soc. **55**, 1817 (1959).
[4] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).

No. 131 Carbonyl bromide $COBr_2$
Symmetry C_{2V} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a_1	ν_1	CO stretch.	1828 B	1828 VS		
	ν_2	CBr_2 s-stretch.	425 C	425 M	429 S	
	ν_3	CBr_2 deform.	181 D		181 S	
b_1	ν_4	CBr_2 a-stretch.	757 C	787 VS		
				747 VS		FR($\nu_2+\nu_5$).
	ν_5	CO deform.	350 C	350 VW	350 M, b	
b_2	ν_6	Op-deform.	512 B	512 M		

References

[1] IR.R. J. Overend and J. C. Evans, Trans. Faraday Soc. **15**, 1817 (1959).
[2] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).

No. 132 Thiocarbonyl fluoride SCF_2
Symmetry C_{2v} **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CS stretch.	1368 C	1368 VS		
	ν_2	CF_2 s-stretch.	787 C	787 M		
	ν_3	CF_2 scis.	526 C	526 M		
b_1	ν_4	CF_2 a-stretch.	1189 C	1189 S		
	ν_5	CF_2 rock.	417 C	417 VW		
b_2	ν_6	CF_2 wag.	622 C	622 W		

References
[1] IR. A. J. Downs, Spectrochim. Acta **19**, 1165 (1963).
[2] IR. M. J. Hopper, J. W. Russel, and J. Overend, Spectrochim. Acta **28A**, 1215 (1972).

No. 133 Thiocarbonyl chloride $CSCl_2$
Symmetry C_{2v} **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CS stretch.	1137 C	1137 VS	1121 (10)	
	ν_2	CCl_2 s-stretch.	505 C	505 M	496 (5)	
	ν_3	CCl_2 scis.	220 D	220 VW, b	200 (1)	
b_1	ν_4	CCl_2 a-stretch.	816 C	816 VS		
	ν_5	CS deform.	294 C	294	287 (3)	
b_2	ν_6	op-Bend.	473 C	473 W		

References
[1] R. H. W. Thompson, J. Chem. Phys. **6**, 748 (1938).
[2] IR. A. J. Downs, Spectrochim. Acta **19**, 1165 (1963).
[3] IR. M. J. Hopper, J. W. Russell, and J. Overend, Spectrochim. Acta **28A**, 1215 (1972).

No. 134 Isocyanic acid HNCO
Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	NH stretch.	3531 C	3531 S	3410	
	ν_2	CO stretch.	2274 C	2274 VS		
	ν_3	CN stretch.	1327 C	1327 W	1318	
	ν_4	NH bend.	762 B[a]	777.1 S		
	ν_5	NCO deform.	643 B[a]	659.8 M		
a''	ν_6	NCO deform.	610 B[a]	577.5 M		

[a] Three fundamentals, ν_4, ν_5, and ν_6, are strongly coupled through Coriolis interaction. The unperturbed frequencies are given in this column [3].

References
[1] R. G. Herzberg and C. Reid, Disc. Faraday Soc. **9**, 92 (1950).
[2] IR. C. Reid, J. Chem. Phys. **18**, 1544 (1954).
[3] IR. R. A. Ashby and R. L. Werner, J. Mol. Spectry. **18**, 184 (1965).

No. 135 Isocyanic acid–d DNCO
Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	ND stretch.	2621 B	2620.7		
	ν_2	CO stretch.	2235 C	2235		
	ν_3	CN stretch.	1310 C	1310		
	ν_4	ND bend.	758 C[a]	766.8		
	ν_5	CNO deform.	458 C[a]	460		
a''	ν_6	CNO deform.	603 B[a]	602.9		

[a] See footnote of HNCO.

References
[1] IR. R. A. Ashby and R. L. Werner, Spectrochim. Acta **22**, 1345 (1966).
[2] IR. W. D. Sheasley, C. W. Mthews, E. L. Ferretti, K. N. Rao, J. Mol. Spectry. **37**, 377 (1971).

No. 136 Carbonyl chlorofluoride COClF

Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CO stretch.	1868 C	1876 VS	1858 M	FR($\nu_2+\nu_3$).
				1847 VS	1832 M	
	ν_2	CF stretch.	1095 B	1095 S	1085 VW	
	ν_3	CCl stretch.	776 C	776 M	765 VS	
	ν_4	CO deform.	501 C	501 W	506 S	
	ν_5	CClF deform.	415 C	415 VW	410 M	
a''	ν_6	Op–deform.	667 B	667 M	665 VW	

References

[1] IR.R. A. H. Nielsen, T. G. Burke, P. J. H. Woltz, and E. A. Jones, J. Chem. Phys. **20**, 596 (1952).
[2] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).

No. 137 Carbonyl bromochloride COBrCl

Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CO stretch.	1828 B	1828 VS		
	ν_2	CCl stretch.	806 C	806 VS		
	ν_3	CBr stretch.	517 C	517 M	518 M	
	ν_4	CO deform.	374 C	374 W	372 M	
	ν_5	CBrCl deform.	240 D		240 S	
a''	ν_6	Op–deform.	547 B	547 W		

References

[1] IR.R. J. Overend and J. C. Evans, Trans. Faraday Soc. **55**, 1817 (1959).
[2] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).

No. 138 Thiocarbonyl bromochloride CSBrCl
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CS stretch.	1130 C	1130 S	1125 W, p	
	ν_2	CCl stretch.	764 C	764 S	761 W	
	ν_3	CBr stretch.	438 C	438 M	437 S, p	
	ν_4	CBrCl deform.	256 D	256 W (liquid)	257 M, p	
	ν_5	CS deform.	222 D	222 VW (liquid)	222 M, p	
a''	ν_6	op–Bend.	405 E			CF [1].

Reference
[1] IR.R.Th. J. L. Brema and D. C. Moule, Spectrochim. Acta **28A**, 809 (1972).

No. 139 Trifluoromethane-d CDF_3
Symmetry C_{3V} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD stretch.	2261 B	2261.0 S		
	ν_2	CF_3 s–stretch.	1111 B	1110.6 M		
	ν_3	CF_3 s–deform.	694 B	694.2 M		
e	ν_4	CD bend.	1202 D	1202.2 M		FR(ν_3+ν_6).
	ν_5	CF_3 d–stretch.	975 B	975.1 S		
	ν_6	CF_3 d–deform.	502 B	502.4 M		

References
[1] IR. S. R. Polo and M. K. Wilson, J. Chem. Phys. **21**, 1129 (1953).
[2] IR. C. C. Costain, J. Mol. Spectry. **9**, 317 (1962).
[3] IR.Th. A. Ruoff, H. Bürger, and S. Biedermann, Spectrochim. Acta **27A**, 1359 (1971).

No. 140 Chlorotrifluoromethane $CClF_3$
Symmetry C_{3V} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CF_3 s-stretch.	1105 C	1105 VS	1106 W, p	
	ν_2	CCl stretch.	781 C	781 S	781.7 VS, p	
	ν_3	CF_3 s-deform.	476 C		475.8 S, p	
e	ν_4	CF_3 d-stretch.	1212 C	1212 VS	1217 W, dp	
	ν_5	CF_3 d-deform.	563 C	563 M	560 W, dp	
	ν_6	CCl bend.	350 C		350 M, dp	

References

[1] IR. H. W. Thompson and R. B. Temple, J. Chem. Soc. **1948**, 1422.
[2] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS **47**, 202 (1951).
[3] R. H. H. Claassen, J. Chem. Phys. **22**, 50 (1954).
[4] R. W. Holzer and H. Moser, J. Mol. Spectry. **20**, 188 (1966).
[5] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 141 Bromotrifluoromethane $CBrF_3$
Symmetry C_{3V} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CF_3 s-stretch.	1089 C	1089 VS	1082 (8) p	
	ν_2	CF_3 s-deform.	760 C	760 VS	761 (9) p	
	ν_3	CBr stretch.	349 C	350[a]	349 (7) p	
e	ν_4	CF_3 d-stretch.	1210 C	1210 VS	1207 (8) dp	
	ν_5	CF_3 d-deform.	547 C	547 M	541 (2) dp	
	ν_6	CBr bend.	306 C	297[a]	306 (2) dp	

[a] Estimated from overtone and combination bands.

References

[1] IR.R. W. F. Edgell and C. E. May, J. Chem. Phys. **20**, 1822 (1952).
[2] IR. E. K. Plyler and N. Acquista, J. Res. NBS **48**, 92 (1952).
[3] IR. P. R. McGee, F. F. Cleveland, A. G. Meister, C. E. Decker, and S. I. Miller, J. Chem. Phys. **21**, 242 (1953).
[4] R. W. Holzer, J. Mol. Spectry. **25**, 123 (1968).
[5] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 142 Trifluoroiodomethane CF_3I

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CF_3 s-stretch.	1080 C	1080 VS	1056	
	ν_2	CF_3 s-deform.	742 C	742 VS	741	
	ν_3	CI stretch.	286 E	286[a]	284[a]	
e	ν_4	CF_3 d-stretch.	1187 C	1187 VS	1168	
	ν_5	CF_3 d-deform.	537 C	537	537	
	ν_6	CI bend.	260 E	260[a]	260[a]	

[a] Estimated from overtone and combination bands.

References

[1] IR.R. W. F. Edgell and C. E. May, J. Chem. Phys. **20**, 1822 (1952).
[2] IR. E. K. Plyler and N. Acquista, J. Res. NBS **48**, 92 (1952).
[3] IR. P. R. McGee, F. F. Cleveland, A. G. Meister, C. E. Decker, and S. I. Miller, J. Chem. Phys. **21**, 242 (1953).
[4] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 143 Trichlorofluoromethane CCl_3F

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CF stretch.	1085 C	1085 S	1090 VW, p	
	ν_2	CCl_3 s-stretch.	535 C	535 M	535 VS, p	
	ν_3	CCl_3 s-deform.	350 C	350 VS	349.5 S, p	
e	ν_4	CCl_3 d-deform.	847 C	847 VS	847 M, dp	
	ν_5	CF bend.	394 C	401 VW	394 S, dp	
	ν_6	CCl_3 d-deform.	241 C		241 S, dp	

References

[1] IR. H. W. Thompson and R. B. Temple, J. Chem. Soc. **1948**, 1422.
[2] R. J. P. Zietlow, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. **18**, 1076 (1950).
[3] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS **47**, 202 (1951).
[4] IR. J. P. Zietlow and F. F. Cleveland, J. Chem. Phys. **21**, 1778 (1951).
[5] R. H. H. Claassen, J. Chem. Phys. **22**, 50 (1954).
[6] R. W. Holzer and H. Moser, J. Mol. Spectry. **20**, 188 (1966).
[7] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 144 Trichloroiodomethane CCl_3I

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	CCl_3 s-stretch.	684 D	684 VS	687 W, b, p	
	ν_2	CI stretch.	390 D	390 M	405 W, p	
	ν_3	CCl_3 s-deform.	224 D	224 W	224 W	
e	ν_4	CCl_3 d-stretch.	755 D	755 VS		
	ν_5	CCl_3 d-deform.	284 D	284 W	288 W, dp	
	ν_6	CI bend.	188 D	188 M		

Reference

[1] IR.R. R. H. Mann and P. M. Manis, J. Mol. Spectry. **45**, 65 (1973).

No. 145 Tribromofluoromethane CBr_3F

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	CF stretch.	1069 D		1069 p	
	ν_2	CBr_3 s-stretch.	398 D		398 p	
	ν_3	CBr_3 s-deform.	218 D		218 p	
e	ν_4	CBr_3 d-stretch.	743 D		743 dp	
	ν_5	CF bend.	306 D		306 dp	
	ν_6	CBr_3 d-deform.	150 D		150 dp	

References

[1] R. M. L. Delwaulle and M. F. François, Comptes Rendus **214**, 828 (1942).
[2] R. M. L. Delwaulle and M. F. François, J. Phys. (Paris) **7**, 15 (1946).
[3] Th. A. G. Meister, S. E. Rosson, and F. F. Cleveland, J. Chem. Phys. **18**, 346 (1950).
[4] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 146 Dichlorodifluoromethane CCl_2F_2

Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CF_2 s-stretch.	1101 C	1101 S	1098 M	
	ν_2	CCl_2 s-stretch.	667 C	667 S	667.2 S, p	
	ν_3	CF_2 scis.	458 D		457.5 S	
	ν_4	CCl_2 scis.	262 C		261.5 S, dp	
a_2	ν_5	CF_2 twist.	322 C	ia	322 W, dp	
b_1	ν_6	CF_2 a-stretch.	1159 C	1159 S	1167 W, dp	
	ν_7	CF_2 rock.	446 C	446 W		
b_2	ν_8	CCl_2 a-stretch.	902 E	922 VS	923 W, dp	
				882 VS		FR($\nu_3+\nu_9$).
	ν_9	CF_2 wag.	437 C	437 W	433 M	

References

See No. 143(CCl_3F).

No. 147 Dibromodifluoromethane CBr_2F_2

Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CF_2 s-stretch.	1090 C	1090	1077 W, p	
	ν_2	CF_2 scis.	623 C	623	624 W, p	
	ν_3	CBr_2 s-stretch.	340 D		340 S, p	
	ν_4	CBr_2 scis.	168 D		168 M, p	
a_2	ν_5	CF_2 twist.	281 D	ia	281 W, dp	
b_1	ν_6	CF_2 a-stretch.	1153 C	1153 VS	1141 VW, dp	
	ν_7	CF_2 rock.	369 D		369 VW, dp	
b_2	ν_8	CBr_2 a-stretch.	831 C	831 VS	816 W, dp	
	ν_9	CF_2 wag.	325 D		325 VW, dp	

References

[1] R. G. Glockler and G. R. Leader, J. Chem. Phys. **7**, 553 (1939).
[2] IR. E. K. Plyler and N. Acquista, J. Res. NBS **48**, 92 (1952).
[3] IR. C. E. Decker and F. F. Cleveland, J. Chem. Phys. **21**, 189 (1953).
[4] IR.R. C. E. Decker, A. G. Meister, F. F. Cleveland, and R. B. Bernstein, J. Chem. Phys. **21**, 1781 (1953).
[5] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 148 **Bromodichlorofluoromethane $CBrCl_2F$**
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CF stretch.	1080 C	1080 VS	1070 (3) p	
	ν_2	CCl_2 s-stretch.	796 C	796 VS	783 (12) p	
	ν_3	CBr stretch.	502 C	502 M (liquid)	504 (100) p	
	ν_4	CCl_2 scis.	339 D		339 (14) p	
	ν_5	CBrF scis.	306 D		306 (98) p	
	ν_6	CCl_2 wag.	218 D		218 (53) p	
a''	ν_7	CCl_2 a-stretch.	838 C	838 VS	831 (5) dp	
	ν_8	CCl_2 twist.	392 D		392 (10) dp	
	ν_9	CCl_2 rock.	204 D		204 (34) dp	

References

[1] R. M. L. Delwaulle and F. François, Comptes Rendus **214**, 828 (1942).
[2] IR.R. R. L. Gilbert, E. A. Piotrowski, J. M. Dowing, and F. F. Cleveland, J. Chem. Phys. **31**, 1633 (1959).
[3] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 149 **Dibromochlorofluoromethane CBr_2ClF**
Symmetry C_S **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CF stretch.	1075 C	1075 VS	1059 (2) p	
	ν_2	CCl stretch.	806 E	795 VS	793 (4) p	
				814 VS	815 (5) p	FR($\nu_3+\nu_4$).
	ν_3	CBr_2 s-stretch.	460 C	460 W (liquid)	464 (58) p	
	ν_4	CClF scis.	341 D		341 (17) p	
	ν_5	CBr_2 scis.	268 D		268 (100) p	
	ν_6	CBr_2 wag.	162 D		162 (50) p	
a''	ν_7	CBr_2 a-stretch.	754 C	754 VS	742 (11) dp	
	ν_8	CBr_2 twist.	308 D		308 (6) dp	
	ν_9	CBr_2 rock.	196 D		196 (20) dp	

References

See No. 148($CBrCl_2F$).

No. 150 Borine Carbonyl $^{10}BH_3CO$

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	BH_3 s-stretch.	2387 D	2387 M (solid)		
	ν_2	CO stretch.	2166 D	2166.0 VS		
	ν_3	BH_3 s-deform.	1083 C	1083.1 S		
	ν_4	BC stretch.	707 B	707.0 S		
e	ν_5	BH_3 d-stretch.	2456 D	2456 VS		
	ν_6	BH_3 d-deform.	1115 E	1114.8 S		
	ν_7	BH_3 rock.	819 B	818.8 M		
	ν_8	BCO bend.	314 B	313.7 S		

References

[1] IR. R. D. Cowan, J. Chem. Phys. **18**, 1101 (1950).
[2] IR.Th. G. W. Bethke and M. K. Wilson, J. Chem. Phys. **26**, 1118 (1957).

No. 151 Borine Carbonyl-d_3 $^{10}BD_3CO$

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	BD_3 s-stretch.	1695 C	1694.8 M		
	ν_2	CO stretch.	2169 D	2169.0 VS		
	ν_3	BD_3 s-deform.	888 D	888.4 W (solid)		
	ν_4	BC stretch.	630 B	629.5 S		
e	ν_5	BD_3 d-stretch.	1852 C	1852 S		
	ν_6	BD_3 d-deform.	802 B	801.5 W		
	ν_7	BD_3 rock.	718 B	718.0 S		
	ν_8	BCO bend.	266 B	266.0 S		

References

See No. 150($^{10}BH_3CO$).

No. 152 Borine Carbonyl $^{11}BH_3CO$
Symmetry C_{3V} Symmetry number σ = 3

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a_1	ν_1	BH_3 s–stretch.	2380 C	2379 M (solid)	2380 S, p	
	ν_2	CO stretch.	2165 D	2164.7 VS	2169 S, p	
	ν_3	BH_3 s–deform.	1073 C	1073.4 S	1073 S, p	
	ν_4	BC stretch.	691 B	691.4 S	692 W, p	
e	ν_5	BH_3 d–stretch.	2444 D	2444 VS	2434 S	
	ν_6	BH_3 d–deform.	1106 E	1105.8 S	1101 M	
	ν_7	BH_3 rock.	809 B	809.3 M	816 W	
	ν_8	BCO bend.	313 B	313.2 S	317 M	

References

[1] IR. R. D. Cowan, J. Chem. Phys. **18**, 1101 (1950).
[2] IR.Th. G. W. Bethke and M. K. Wilson, J. Chem. Phys. **26**, 1118 (1957).
[3] R.Th. R. C. Taylor, J. Chem. Phys. **26**, 1131 (1957).

No. 153 Borine Carbonyl–d_3 $^{11}BD_3CO$
Symmetry C_{3V} Symmetry number σ = 3

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a_1	ν_1	BD_3 s–stretch.	1679 C	1679.0 M	1678 S	
	ν_2	CO stretch.	2169 D	2168.5 VS	2169 S	
	ν_3	BD_3 s–deform.	860 C	867.7 W (solid)	860 M	
	ν_4	BC stretch.	625 B	624.8 S	619 M	
e	ν_5	BD_3 d–stretch.	1840 C	1840 S	1825 S	
	ν_6	BD_3 d–deform.	801 B	801.3 W	808 M	
	ν_7	BD_3 rock.	709 B	709.3 S	706 W	
	ν_8	BCO bend.	266 B	266.0 S	264 W	

References

See No. 152($^{11}BH_3CO$).

No. 154 Methylmercuric iodide CH_3HgI
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected frequency value of	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Solid)	cm^{-1} (CH_3NO_2 soln.)	
a_1	ν_1	CH_3 s-stretch.	2920 D	2920 M	2914 (Solid)	
	ν_2	CH_3 s-deform.	1180 D	1180 M	1182 p	
	ν_3	CHg stretch.	531 D	531 M	538 p	
	ν_4	HgI stretch.	184 D	184 M	180 p	
e	ν_5	CH_3 d-stretch.	3008 D	3008 M		
	ν_6	CH_3 d-deform.	1400 D	1400 W		
	ν_7	CH_3 rock.	781 D	781 S		
	ν_8	CHgI bend.	64 D	64 M		

References
[1] R. F. Fehéh, W. Kolb and L. Leverenz, Z. Naturforsch., A **2**, 454 (1947).
[2] IR.R. P. L. Goggin and L. A. Woodward, Trans. Faraday Soc. **62**, 1423 (1966).
[3] IR.Th. J. H. S. Green, Spectrochim. Acta **24A**, 863 (1968).

No. 155 Methylsilane CH_3SiH_3
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s-stretch.	2898 E	2928.8 M 2867.4 M		FR(ν_2+ν_5).
	ν_2	SiH_3 s-stretch.	2169 C	2169 S		
	ν_3	CH_3 s-deform.	1260 C	1260 M		
	ν_4	SiH_3 s-deform.	940 C	940 VS		
	ν_5	CSi stretch.	700 C	700 S		
a_2	ν_6	Torsion	187 D	ia		187.6(A). MW. 186.9(E).
e	ν_7	CH_3 d-stretch.	2982 A	2981.6 M		
	ν_8	SiH_3 d-stretch.	2166 A	2965.7 S		
	ν_9	CH_3 d-deform.	1403 C	1403 M		
	ν_{10}	SiH_3 d-deform.	980 D	980[a]		
	ν_{11}	CH_3 rock.	868 B	867.5 S		
	ν_{12}	SiH_3 rock.	540 C	540 M		

[a] The band origin is not determined clearly.

References
[1] IR. S. Kaye and S. Tannnenbaum, J. Org. Chem. **18**, 1750 (1953).
[2] IR. D. F. Ball, P. L. Goggin, D. C. McKean, and L. A. Woodward, Spectrochim. Acta **16**. 1358 (1960).
[3] IR. R. E. Wilde, J. Mol. Spectry. **8**, 427 (1962).
[4] IR. M. Randie, Spectrochim. Acta **18**, 115 (1962).
[5] Th. E. A. Clark and A. Weber, J. Chem. Phys. **45**, 1759 (1966).

No. 156 Methylsilane-d$_3$ CH_3SiD_3
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s-stretch.	2923 A	2923.4 M		
	ν_2	Sid_3 s-stretch.	1558 C	1558 M		
	ν_3	CH_3 s-deform.	1262 C	1262 S		
	ν_4	CSi stretch.	741 C	741 VS		
	ν_5	SiD_3 s-deform.	652 C	652 S		
a_2	ν_6	Torsion	172 D	ia		172.1(A) MW. 171.9(E)
e	ν_7	CH_3 d-stretch.	2982 A	2981.8 M		
	ν_8	SiD_3 d-stretch.	1577 C	1577 VS		
	ν_9	CH_3 d-deform.	1401 C	1401 M		
	ν_{10}	CH_3 rock.	825 C	825 S		
	ν_{11}	SiD_3 d-deform.	668 C	668 S		
	ν_{12}	SiD_3 rock.	433 C	433		

References
[1] IR. D. E. Ball, P. L. Goggin, D. C. McKean, and L. A. Woodward, Spectrochim. Acta **16**, 1358 (1960).
[2] IR. R. E. Wilde, J. Mol. Spectry. **8**, 427 (1962).
[3] Th. E. A. Clark and A. Weber, J. Chem. Phys. **45**, 1759 (1966).

No. 157 Methylgermane CH_3GeH_3
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s-stretch.	2938 B	2937.8 S		
	ν_2	GeH_3 s-stretch.	2085 B	2084.8 S		
	ν_3	CH_3 s-deform.	1254 B	1254.1 M		
	ν_4	GeH_3 s-deform.	843 B	842.5 VS		
	ν_5	CGe stretch.	602 B	601.6 VS		
a_2	ν_6	Torsion	157 D	ia		158.1(A) MW. 156.1(E)
e	ν_7	CH_3 d-stretch.	2997 B	2997.2 S		
	ν_8	GeH_3 d-stretch.	2084 B	2084.3 S		
	ν_9	CH_3 d-deform.	1428 C	1427.7 W		
	ν_{10}	GeH_3 d-deform.	900 C	900.4 S		
	ν_{11}	CH_3 rock.	848 C	847.5 S		
	ν_{12}	GeH_3 rock.	506 C	505.9 S		

References
[1] IR. J. E. Griffiths, J. Chem. Phys. **38**, 2879 (1963).
[2] Th. E. A. Clark and A. Weber, J. Chem. Phys. **45**, 1759 (1966).

No. 158 Methyl-d$_3$-germane CD_3GeH_3
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 s-stretch.	2090 C	2091.0 S		
	ν_2	GeH_3 s-stretch.	2073 C	2073 S		
	ν_3	CD_3 s-deform.	978 C	977.5 S		
	ν_4	GeH_3 s-deform.	844 C	844.3 S		
	ν_5	CGe stretch.	550 B	549.6 S		
a_2	ν_6	Torsion	132 D	ia		131.7(A) MW. 131.5(E)
e	ν_7	CD_3 d-stretch.	2248 B	2247.5 S		
	ν_8	GeH_3 d-stretch.	2089 B	2089.0 S		
	ν_9	CD_3 d-deform.	1032 B	1032.0 M		
	ν_{10}	GeH_3 d-deform.	904 B	903.9 S		
	ν_{11}	CD_3 rock.	713 C	713 S		
	ν_{12}	GeH_3 rock.	452 B	451.8 S		

References
See No. 157(CH_3GeH_3).

No. 159 Methyltriiodogermane CH_3GeI_3
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 s-stretch.	2911 C	2911 M	2909 W	
	ν_2	CH_3 s-deform.	1225 C	1225 M	1222 W	
	ν_3	CGe stretch.	597 C	597 S	596 M	
	ν_4	GeI_3 s-stretch.	195 C	196 M (Solid)	195 S	
	ν_5	GeI_3 s-deform.	92 C	96 M (Solid)	92 S	
a_2	ν_6	Torsion	123 D	123 Vw (Solid)	123 Vw	
e	ν_7	CH_3 d-stretch.	2999 C	2999 M	2996 W	
	ν_8	CH_3 d-deform.	1392 C	1392 S	1394 (Solid)	
	ν_9	CH_3 rock.	810 C	810 S	809 (Solid)	
	ν_{10}	GeI_3 d-stretch.	252 C	252 S	251 M	
	ν_{11}	GeI_3 rock.	147 C		147 M	
	ν_{12}	GeI_3 d-deform.	67 C		67 S	

References
[1] IR. R. J. Cross and F. Glockling, J. Organometal. Chem. **3**, 146 (1965).
[2] IR.R.Th. J. R. Durig, C. F. Jumper, and J. N. Willis, Jr., J. Mol. Spectry. **37**, 260 (1971).

No. 160 Methylstannane CH_3SnH_3
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s-stretch.	2933 B	2932.5 W		
	ν_3	CH_3 s-deform.	1209 B	1209.3 W		
	ν_2	SnH_3 s-stretch.	1875 D	1874.5 S		OV(ν_8).
	ν_4	SnH_3 s-deform.	695 B	694.5 S		
	ν_5	SnC stretch.	527 B	526.9 M		
a_2	ν_6	Torsion	109 C			MW[1].
e	ν_7	CH_3 d-stretch.	3005 B	3005.4 W		
	ν_8	SnH_3 d-stretch.	1875 B	1874.5 S		OV(ν_2).
	ν_9	CH_3 d-deform.	1417 B	1417.0 W		
	ν_{10}	CH_3 rock.	774 C	774.1 M		
	ν_{11}	SnH_3 d-deform.	741 C	741.3 M		
	ν_{12}	SnH_3 rock.	416 B	416.3 M		

References
[1] MW. P. Cahill and S. Butcher, J. Chem. Phys. **35**, 2255 (1961).
[2] IR. H. Kimmel and C. R. Dillard, Spectrochim. Acta **24A**, 909 (1968).

No. 161 Methylstannane-d_3 CH_3SnD_3
Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s-stretch.	2930 D	2930 M		
	ν_2	SnD_3 s-stretch.	1352 D	1352.0 S		OV(ν_9).
	ν_3	CH_3 s-deform.	1205 C	1204.5 S		
	ν_4	SnC stretch.	509 C	509.1 M		
	ν_5	SnD_3 s-deform.	493 C	493.0 S		
a_2	ν_6	Torsion	101 C			MW[1].
e	ν_7	CH_3 d-stretch.	3000 D	3000 W		
	ν_8	CH_3 d-deform.	1400 D	1400 W		
	ν_9	SnD_3 d-stretch.	1352 C	1352.0 S		OV(ν_2).
	ν_{10}	CH_3 rock.	765 D	765 W		
	ν_{11}	SnD_3 d-deform.	503 C	502.5 S		
	ν_{12}	SnD_3 rock.	317 D	316.6 M		

References
See No. 160(CH_3SnH_3).

No. 162 Methyl-d$_3$-stannane CD_3SnH_3

Symmetry C_{3v} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 s-stretch.	2144 B	2144.3 M		
	ν_2	SnH_3 s-stretch.	1889 D	1889.0 S		OV(ν_8).
	ν_3	CD_3 s-deform.	920 B	920.2 M		
	ν_4	SnH_3 s-deform.	704 B	703.5 S		
	ν_5	SnC stretch.	478 B	478.0 M		
a_2	ν_6	Torsion	88 C			MW[1].
e	ν_7	CD_3 d-stretch.	2255 C	2254.5 M		
	ν_8	SnH_3 d-stretch.	1889 B	1889.0 S		OV(ν_2).
	ν_9	CD_3 d-deform.	1017 C	1017.1 W		
	ν_{10}	SnH_3 d-deform.	738 B	738.1 M		
	ν_{11}	CD_3 rock.	628 B	628.4 S		
	ν_{12}	SnH_3 rock.	392 C	392.4 W		

References

See No. 160(CH_3SnH_3).

No. 163 Cyanogen C_2N_2

Symmetry $D_{\infty h}$ **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	CN s-stretch.	2330 B	2339.9[a]	2330.5	
	ν_2	NN stretch.	846 C	ia	845.5	
σ_u^+	ν_3	CN a-stretch.	2158 A	2157.83	ia	
π_g	ν_4	CCN bend.	503 C	ia	502.8	
π_u	ν_5	CCN bend.	234 B	233.1[a]	233.7	

[a] Determined from difference bands[3].

References

[1] R. A. Langseth and C. K. Moller, Acta Chem. Scand. **4**, 725 (1950).
[2] IR. G. D. Craine and H. W. Thompson, Trans. Faraday Soc. **49**, 1273 (1953).
[3] IR. A. G. Maki, J. Chem. Phys. **43**, 3193 (1965).
[4] Th. W. Sawodnt and A. Ruoff, J. Mol. Spectry. **34**, 173 (1970).
[5] R.IR.Th. L. J. Jones, J. Mol. Spectry. **45**, 55 (1973).
[6] IR. M. A. Picard, Spectrochim. Acta **29**, 423 (1973).
[7] R.Th. L. H. Jones, J. Mol. Spectry. **49**, 82 (1974).

No. 164 Dichloroacetylene C_2Cl_2

Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
σ_g^+	ν_1	CC stretch.	2234 D	ia	2234 S, p	
	ν_2	CCl stretch.	477 D	ia	477 M, p	
σ_u^+	ν_3	CCl stretch.	988 C	988 VS	ia	
π_g	ν_4	CCCl deform.	333 D	ia	333 VS, dp	
π_u	ν_5	CCCl deform.	172 C	172 S	ia	

Reference

[1] IR.R. P. Klaboe and E. Kloster–Jensen, Spectrochim. Acta **26A**, 1567 (1970).

No. 165 Dibromoacetylene C_2Br_2

Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (C_6H_6 soln.)	
σ_g^+	ν_1	CC stretch.	2185 D	ia	2185 VS, p	
	ν_2	CBr stretch.	267 D	ia	267 M, p	
σ_u^+	ν_3	CBr stretch.	832 C	832 VS	ia	
π_g	ν_4	CCBr deform.	311 D	ia	311 VS, dp	
π_u	ν_5	CCBr deform.	137 C	137 S	ia	

Reference

See No. 164(C_2Cl_2).

No. 166 Diiodoacetylene C_2I_2

Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1}	cm^{-1} (C_6H_6 soln.)	
σ_g^+	ν_1	CC stretch.	2118 D	ia	2118 VS, p	
	ν_2	CI stretch.	190 D	ia	190 S, p	
σ_u^+	ν_3	CI stretch.	720 D	720 VS (CS_2 soln.)	ia	
π_g	ν_4	CCI deform.	296 D	ia	296 VS, dp	
π_u	ν_5	CCI deform.	132 D	132 M (C_6H_6 soln.)	ia	

References

[1] IR.R. A. G. Meister and F. F. Cleveland, J. Chem. Phys. **17**, 212 (1949).
[2] IR.R. P. Klaboe and E. Kloster–Jensen, Spectrochim Acta **26A**, 1567 (1970).

No. 167 Bromochloroacetylene C_2BrCl
Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (C_6H_6 soln.)	
σ^+	ν_1	CC stretch.	2223 C	2223 VS	2205 M, p	
	ν_2	CCl stretch.	923 C	923 VS	917 VS	
	ν_3	CBr stretch.	389 C	389 VW	388 S, p (CCl_4 soln.)	
π	ν_4	CCCl deform.	326 D		326 VS, dp (CCl_4 soln.)	
	ν_5	CCBr deform.	152 C	152 S	165 M	

Reference
See No. 164(C_2Cl_2).

No. 168 Chloroiodoacetylene C_2ClI
Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (C_6H_6 soln.)	
σ^+	ν_1	CC stretch.	2191 C	2191 VS	2178 VS, p	
	ν_2	CCl stretch.	886 C	886 VS	880 VW	
	ν_3	CI stretch.	276 D		276 M, p	
π	ν_4	CCCl deform.	325 D		325 VS, dp	
	ν_5	CCI deform.	135 C	135 S	145 VW (CCl_4 soln.)	

Reference
See No. 167(C_2ClBr).

No. 169 Bromoiodoacetylene C_2BrI
Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (CS_2 soln.)	
σ^+	ν_1	CC stretch.	2166 B	2166 S	2153 VS	
	ν_2	CBr stretch.	782 C	782 M	775 VW	
	ν_3	CI stretch.	222 D		222 M, p	
π	ν_4	CBr bend.	304 D		304 VS, dp	
	ν_5	CI bend.	122 B	122 S		

Reference

[1] IR.R. D. H. Christensen, T. Stroger–Hansen, P. Klaboe, E. Kloster–Jensen, and E. E. Tucker, Spectrochim. Acta **28A**, 939 (1972).

No. 170 Trifluoroacetonitrile CF_3CN
Symmetry C_{3V} **Symmetry number σ = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CN stretch.	2275 B	2275.0	2274 S, p	
	ν_2	CF_3 s–stretch.	1227 B	1227.2	1222 VW	
	ν_3	CC stretch.	802 B	801.7	818 M, p	
	ν_4	CF_3 s–deform.	522 B	521.8	521 M, p	
e	ν_5	CF_3 d–stretch.	1214 B	1214.3	1192 W	
	ν_6	CF_3 d–deform.	618 B	618.3	620 W, dp	
	ν_7	CF_3 rock.	463 B	462.7	463 W, dp	
	ν_8	CCN deform.	196 B	196.0	192 S, dp	

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[1] IR.R. W. F. Edgell and R. M. Potter, J. Chem. Phys. **24**, 80 (1956).
[2] IR. J. A. Faniran and H. F. Shurvell, Spectrochim. Acta **26A**, 1459 (1970).
[3] IR.Th. J. A. Faniran and H. F. Shurvell, Spectrochim. Acta **27A**, 1945 (1971).

No. 171 trans-1,2-Difluoroethylene CHFCHF
Symmetry C_{2h} **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a_g	ν_1	CH stretch.	3111 C	ia	3111 VS, p	
	ν_2	CC stretch.	1694 C	ia	1694 VS, p	
	ν_3	CH bend.	1286 C	ia	1286 S, p	
	ν_4	CF stretch.	1123 C	ia	1123 M, p	
	ν_5	CCF deform.	548 C	ia	548 S, p	
a_u	ν_6	CH bend.	875 B	875 S	ia	
	ν_7	Torsion	329 D	333 M (Xe Matrix) 325 M (Xe Matrix)	ia	
b_g	ν_8	CH bend.	788 C	ia	788 S, dp	
b_u	ν_9	CH stretch.	3114 C	3114 M	ia	
	ν_{10}	CH bend.	1274 C	1274 M	ia	
	ν_{11}	CF stretch.	1159 C	1159 VS	ia	
	ν_{12}	CCF deform.	341 D	341 M (Xe Matrix)	ia	

Reference

[1] IR.R. N. C. Craig and J. Overend, J. Chem. Phys. **51**, 1127 (1969).

No. 172 trans-1,2-Difluoroethylene-d₁ CHFCDF
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a'	ν_1	CH stretch.	3110 C	3110 M	3112 S, p	
	ν_2	CD stretch.	2335 C	2335 M	2333 M, p	
	ν_3	CC stretch.	1674 C		1674 S, p	
	ν_4	CH bend.	1274 C	1274 M	1274 M, p	
	ν_5	CF stretch.	1166 C	1166 VS	1155 VW	
	ν_6	CF stretch.	1138 C	1138 M	1119 M, p	
	ν_7	CD bend.	940 C	940 M	941 M, dp	
	ν_8	CCF deform.	542 C		542 S, p	
	ν_9	CCF deform.	332 D	332 M		
a''	ν_{10}	CH bend.	828 B	828 S	829 M, dp	
	ν_{11}	CD bend.	673 B	673 M	673 M, dp	
	ν_{12}	Torsion	316 C	316 S		

Reference

See No. 171(CHFCHF).

No. 173 trans-1,2-Difluoroethylene-d_2 CDFCDF
Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CD stretch.	2355 C	ia	2355 S, p	
	ν_2	CC stretch.	1642 C	ia	1642 VS, p	
	ν_3	CF stretch.	1109 C	ia	1109 S, p	
	ν_4	CD bend.	935 C	ia	935 M, dp	
	ν_5	CCF deform.	538 C	ia	538 S, p	
a_u	ν_6	CD bend.	651 B	651 S	ia	
	ν_7	Torsion	309 C	309 S	ia	
b_g	ν_8	CD bend.	685 C	ia	685 S, dp	
b_u	ν_9	CD stretch.	2312 C	2312 M	ia	
	ν_{10}	CF stretch.	1173 C	1173 VS	ia	
	ν_{11}	CD bend.	942 C	942 M	ia	
	ν_{12}	CCF deform.	324 D	324 M	ia	

References

[1] R. N. C. Craig and J. Overend, Spectrochim. Acta **20**, 1561 (1964).
[2] IR.R. N. C. Craig and J. Overend, J. Chem. Phys. **51**, 1127 (1969).

No. 174 Glyoxal $C_2H_2O_2$
Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_g	ν_1	CH stretch.	2843 B	ia		EL[4].
	ν_2	CO stretch.	1745 B	ia		EL[4].
	ν_3	CH bend.	1338 D	ia		OC[1].
	ν_4	CC stretch.	1065 B	ia		EL[4].
	ν_5	CCO deform.	551 B	ia		EL[3].
a_u	ν_6	CH bend.	801 B	801.36 M		
	ν_7	Torsion	127 B	126.5 W		EL[3].
b_g	ν_8	CH bend.	1048 B	ia		[5].
b_u	ν_9	CH stretch.	2835 B	2835.07 VS		
	ν_{10}	CO stretch.	1732 C	1732 VS		
	ν_{11}	CH bend.	1312 B	1312.38 S		
	ν_{12}	CCO deform.	339 B	338.55 S		

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[1] IR.R. R. K. Harris, Spectrochim. Acta **20**, 1129 (1964).
[2] IR. A. R. H. Cole and G. A. Osborne, J. Mol. Spectry. **36**, 276 (1970).
[3] EL. F. W. Birss, J. M. Brown, A. R. H. Cole, A. Loftus, S. L. N. G. Krishnamachari, G. A. Osborne, J. Puldus, D. A. Ramsay, and L. Watmann, Can. J. Phys. **48**, 1230 (1970).
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[5] IR. A. R. H. Cole and G. A. Osborne, Spectrochim. Acta **27A**, 2461 (1971).

No. 175 Glyoxal-d$_1$ C_2HDO_2
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH stretch.	2835 B	3835.2 S		
	ν_2	CD stretch.	2130 B	2130.2 S		
	ν_3	CO s-stretch.	1735 D	1735 M		
	ν_4	CO a-stretch.	1717 C	1717 VS		
	ν_5	CH bend.	1335 B	1335.0 W		
	ν_6	CC stretch.	1104 E			CF[1].
	ν_7	CD bend.	972 B	971.6 M		
	ν_8	CCO s-deform.	542 D	542[a]		EL[2].
	ν_9	CCO a-deform.	323 B	323.7 S		
a''	ν_{10}	CH bend.	999 D	999 W		
	ν_{11}	CO bend.	688 D			CF.[b]
	ν_{12}	Torsion	124 B	123.9 W		

[a] From the analyses of electronic transitions.
[b] From the product rule.

References

[1] Th. T. Fukuyama, Ph. D. Thesis (University of Tokyo, 1970).
[2] IR. A. R. H. Cole and G. A. Osborne, Spectrochim. Acta **27A**, 2461 (1971).

No. 176 Glyoxal-d$_2$ $C_2D_2O_2$
Symmetry C_{2h} **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_g	ν_1	CD stretch.	2138 D	ia		OC[5].
	ν_2	CO stretch.	1722 C	ia		OC[5].
	ν_3	CD bend.	1130 D	ia		OC[5].
	ν_4	CC stretch.	915 E	ia		CF[3].
	ν_5	CCO deform.	537 B	ia		EL[2].
a_u	ν_6	CD bend.	630 D			CF[1].[a]
	ν_7	Torsion	118 B	118.2 W		EL[2].
b_g	ν_8	CD bend.	911 D	ia		CF[1].[a]
b_u	ν_9	CD stretch.	2130 C	2130 S		
	ν_{10}	CO stretch.	1710 C	1710 VS		
	ν_{11}	CH bend.	1010 B	1010.12 M		
	ν_{12}	CCO deform.	311 B	311.05 M		

[a] From the product rule

References

[1] IR. J. C. D. Brand and G. J. Minkoff, J. Chem. Soc. **1954**, 2970.
[2] EL. J. C. D. Brand, Trans. Faraday Soc. **50**, 431 (1954).
[3] Th. T. Fukuyama, K. Kuchitsu, and Y. Morino, Bull. Chem. Soc. Japan, **41**, 3019 (1968).
[4] EL. D. M. Agar, E. J. Bair, F. W. Birss, P. Bovrell, P. C. Chen, C. N. Gurrie, A. J. Mchugh, B. J. Orr, D. A. Ramsay, and J. Y. Roncin, Can. J. Phys. **49**, 323 (1971).
[5] IR. A. R. H. Cole and G. A. Osborne, Spectrochim. Acta **27A**, 2461 (1971).

No. 177 Acetyl fluoride CH_3COF
Symmetry C_s Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a'	ν_1	CH_3 d-stretch.	3043 C	3043 W	3043 VW	
	ν_2	CH_3 s-stretch.	2955 C	2955 VW	2952 S	
	ν_3	C=O stretch.	1870 C	1870 VS	1847 S	
	ν_4	CH_3 d-deform.	1440 C	1440 W	1440 W	
	ν_5	CH_3 s-deform.	1378 C	1378 M	1379 W	
	ν_6	CF stretch.	1188 C	1188 VS	1178 VW	
	ν_7	CH_3 rock.	1000 C	1000 M	1003 M	
	ν_8	CC stretch.	826 C	826 S	822 S	
	ν_9	OCF deform.	598 C	598 W	602 M	
	ν_{10}	OCF deform.	420 D	420 VW	428 W	
a''	ν_{11}	CH_3 d-stretch.	3004 C	3004 W	3004 VW	
	ν_{12}	CH_3 d-deform.	1437 D	1437 W	1440 W	
	ν_{13}	CH_3 rock.	1054 C	1054 M		
	ν_{14}	C=O op-bend.	567 C	567 W	573 W	
	ν_{15}	CH_3 torsion	123 E			CF[1].

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[1] MW. L. Pierce and L. C. Krisher, J. Chem. Phys. **31**, 875 (1959).
[2] R. H. Seewan–Albert and L. Kahovec, Acta Phys. Austriaca **1**, 352 (1948).
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[4] IR.R. C. V. Berney and A. D. Cormier, Spectrochim. Acta **28A**, 1813 (1972).

No. 178 Acetyl fluoride-d_3 CD_3COF
Symmetry C_s Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a'	ν_1	CD_3 d-stretch.	2274 D	2286 M	2272 W	
				2263 M		FR($\nu_3+\nu_{10}$).
	ν_2	CD_3 s-stretch.	2144 C	2144 W	2140 S	
	ν_3	C=O stretch.	1869 C	1869 VS	1849 M	
	ν_4	CF stretch.	1204 C	1204 VS	1196 VW	
	ν_5	CD_3 s-deform.	1149 C	1149 W		
	ν_6	CD_3 d-deform.	1030 C	1030 S	1030 W	
	ν_7	CD_3 rock.	839 C	839 M	845 M	
	ν_8	CC stretch.	778 C	778 S	774 M	
	ν_9	OCF deform.	575 C	575 M	578 M	
	ν_{10}	OCF deform.	395 D	395 VW	378 W	
a''	ν_{11}	CD_3 d-stretch.	2242 C	2242 W	2250 W	
	ν_{12}	CD_3 d-deform.	1057 C	1057 M	1053 W	
	ν_{13}	CD_3 rock.	915 C	915 M		
	ν_{14}	C=O op-bend.	491 C	491 M	495 W	
	ν_{15}	CD_3 torsion	93 E			CF[1].

References
[1] MW. L. Pierce and L. C. Krisher, J. Chem. Phys. **31**, 875 (1959).
[2] IR. C. V. Berney, R. L. Redington and K. C. Lin, J. Chem. Phys. **53**, 1713 (1970).
[3] IR.R. C. V. Berney and A. D. Cormier, Spectrochim. Acta **28A**, 1813 (1972).

No. 179 Dimethylzinc CH_3ZnCH_3

Symmetry $D_{3h}'(G^{+}_{36})$[a] **Symmetry number σ = 6**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CH_3 s-stretch.	2900 C	ia	2900 S, p	
	ν_2	CH_3 s-deform.	1157 C	ia	1157 S, p	
	ν_3	CZn s-stretch.	503 C	ia	503 VS, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CH_3 s-stretch.	2915 C	2915 S	ia	
	ν_6	CH_3 s-deform.	1183 C	1183 M	ia	
	ν_7	CZn a-stretch.	613 C	613	ia	
e'	ν_8	CH_3 d stretch.	2966 C	2966 S	2947	
	ν_9	CH_3 d-deform.	1301 C	1301 M	1302 W	
	ν_{10}	CH_3 rock.	704 C	704 S		
	ν_{11}	CZnC deform.	134 D		134 sh	
e''	ν_{12}	CH_3 d-stretch.	2843 C	2843	2830	
	ν_{13}	CH_3 d-deform.	1434 C		1434 W	
	ν_{14}	CH_3 rock.	620 C		620 M	

[a] Free rotation [3,5].

References

[1] IR.R. H. S. Gutowsky, J. Chem. Phys. **17**, 128 (1949).
[2] Th.IR. D. R. J. Boyd, R. L. Williams, and H. W. Thompson, Nature **167**, 766 (1951).
[3] IR.R. J.-L. Bribes, Ph. D. Thesis, (Universite des Sciences et Techniques du Languedoc 1971).
[4] Th. A. M. W. Bakke, J. Mol. Spectry. **41**, 1 (1972).
[5] IR.R. J. R. Durig and S. C. Brown, J. Mol. Spectry. **45**, 338 (1973).

No. 180 Dimethylzinc-d_6 CD_3ZnCD_3

Symmetry $D_{3h}'(G^{+}_{36})$[a] **Symmetry number σ = 6**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CD_3 s-stretch.	2109 C	ia	2109 S, p	
	ν_2	CD_3 s-deform.	898 C	ia	898 S, p	
	ν_3	CZn s-stretch.	458 C	ia	458 S, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CD_3 s-stretch.	2117 C	2117 M	ia	
	ν_6	CD_3 s-deform.	934 C	934 M	ia	
	ν_7	CZn a-stretch.	554 C	554 S	ia	
e'	ν_8	CD_3 d-stretch.	2219 C	2219 M	2206 M	
	ν_9	CD_3 d-deform.	960 C	960 W		
	ν_{10}	CD_3 rock.	585 D	585 sh		
	ν_{11}	CZnC deform.	96 D		96 sh	
e''	ν_{12}	CD_3 d-stretch.	2073 C	2073 W	2075 sh	
	ν_{13}	CD_3 d-deform.	1006 C	1006 W		
	ν_{14}	CD_3 rock.	495 C		495 W, p	

[a] Free rotation [1].

Reference

[1] IR.R. J. R. Durig and S. C. Brown, J. Mol. Spectry. **45**, 338 (1973).

No. 181 Dimethylcadmium CH_3CdCH_3

Symmetry $D_{3h}'(G^-_{36})$[a] **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CH_3 s-stretch.	2903 C	ia	2903 S, p	
	ν_2	CH_3 s-deform.	1127 C	ia	1127 S, p	
	ν_3	CCd s-stretch.	459 C	ia	459 S, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CH_3 s-stretch.	2923 C	2923 S	ia	
	ν_6	CH_3 s-deform.	1136 C	1136 M	ia	
	ν_7	CCd a-stretch.	535 C	535 S	ia	
e'	ν_8	CH_3 d-stretch.	2980 C	2980 VS		
	ν_9	CH_3 d-deform.	1315 C	1315	1324	
	ν_{10}	CH_3 rock.	700 C	700 S		
	ν_{11}	CCdC deform.	124 C	124 W	120 W, b	
e''	ν_{12}	CH_3 d-stretch.	2859 C	2859	2834 M	
	ν_{13}	CH_3 d-deform.	1427 C		1427 W	
	ν_{14}	CH_3 rock.	634 C		634 M, dp	

[a] Free rotation [3,5].

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[1] R. F. Fehér, W. Kolb, and L. Leverenz, Z. Naturforsh. **2a**, 454 (1947).
[2] IR. H. S. Gutowsky, J. Amer. Soc. **71**, 3194 (1949).
[3] IR.R. J.-L. Bribes, Ph. D. Thesis, (Universite des Sciences et Techniques du Languedoc 1971).
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[5] IR.R. J. R. Durig and S. C. Brown, J. Mol. Spectry. **45**, 338 (1973).

No. 182 Dimethylcadmium-d_6 CD_3CdCD_3

Symmetry $D_{3h}'(G^-_{36})$[a] **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CD_3 s-stretch.	2112 C	ia	2112 S, p	
	ν_2	CD_3 s-deform.	873 C	ia	873 S, p	
	ν_3	CCd s-stretch.	419 C	ia	419 S, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CD_3 s-stretch.	2120 C	2120 S	ia	
	ν_6	CD_3 s-deform.	900 C	900 W	ia	
	ν_7	CCd a-stretch.	492 C	492 S	ia	
e'	ν_8	CD_3 d-stretch.	2229 C	2229 S	2214 M, dp	
	ν_9	CD_3 d-deform.	1047 D		1047 W	
	ν_{10}	CD_3 rock.	538 C	538 S		
	ν_{11}	CCdC deform.	109 D		109 sh	
e''	ν_{12}	CD_3 d-stretch.	2080 D	2080	2086 sh	
	ν_{13}	CD_3 d-deform.	1126 C		1126	
	ν_{14}	CD_3 rock.	476 C		476 M, dp	

[a] Free rotation [1].

Reference

See No. 180(CD_3ZnCD_3).

No. 183 Dimethylmercury CH_3HgCH_3

Symmetry $D_{3h}'(G^+_{36})$[a] **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CH_3 s-stretch.	2911 C	ia	2911 VS, p	
	ν_2	CH_3 s-deform.	1182 C	ia	1182 VS, p	
	ν_3	CHg s-stretch.	515 C	ia	515 VS, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CH_3 s-stretch.	2925 D	2925 b	ia	
	ν_6	CH_3 s-deform.	1191 C	1191 M	ia	
	ν_7	CHg a-stretch.	540 C	540 VS	ia	
e'	ν_8	CH_3 d-stretch.	2962 C	2962 S		
	ν_9	CH_3 d-deform.	1397 C		1397 W, dp	
	ν_{10}	CH_3 rock.	780 C	780 VS	779 VW, dp	
	ν_{11}	CHgC deform.	161 C		161 M, dp	
e''	ν_{12}	CH_3 d-stretch.	2874 C		2874 S, p	
	ν_{13}	CH_3 d-deform.	1442 C		1442 W, dp	
	ν_{14}	CH_3 rock.	699 C	700 sh	699 M, dp	

[a] Free rotation [3,6].

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[1] IR.R. H. S. Gutowsky, J. Chem. Phys. **17**, 128 (1949).
[2] Th.IR. D. R. J. Boyd, R. L. Williams and H. W. Thompson, Nature **167**, 766 (1951).
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No. 184 Dimethylmercury-d_6 CD_3HgCD_3

Symmetry $D_{3h}'(G^{+}_{36})$[a] **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CD_3 s-stretch.	2111 C	ia	2111 M, p	
	ν_2	CD_3 s-deform.	909 C	ia	909 VS, p	
	ν_3	CHg s-stretch.	471 C	ia	471	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CD_3 s-stretch.	2114 C	2114 S	ia	
	ν_6	CD_3 s-deform.	931 C	931 M	ia	
	ν_7	CHg a-stretch.	491 C	491 VS	ia	
e'	ν_8	CD_3 d-stretch.	2224 C	2224	2224 S, dp	
	ν_9	CD_3 d-deform.	1030 C	1030 M	1030 W, dp	
	ν_{10}	CD_3 rock.	598 C	598 VS		
	ν_{11}	CHgC deform.	141 C		141 S, dp	
e''	ν_{12}	CD_3 d-stretch.	2039 C	2039	2044 M, p	
	ν_{13}	CD_3 d-deform.	1050 C		1050 VW, p	
	ν_{14}	CD_3 rock.	525 C		525 M, sh, dp	

[a] Free rotation [2,4].

References

[1] IR.R. J.-L. Bribes et R. Gaufrès, J. Chim. Phys. **67**, 1168 (1970).
[2] Th. J.-L. Bribes et R. Gaufrès, J. Mol. Structure **9**, 423 (1971).
[3] Th. A. M. W. Bakke, J. Mol. Spectry. **41**, 1 (1972).
[4] Th. J. R. Durig and S. C. Brown, J. Mol. Spectry. **45**, 338 (1973).

No. 185 Azomethane CH_3NNCH_3
Symmetry C_{2h} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CH_3 d-stretch.	2977 C	ia	2977 M, dp	
	ν_2	CH_3 s-stretch.	2916 C	ia	2916 S, p	
	ν_3	NN stretch.	1580 C	ia	1580 VW, p	
	ν_4	CH_3 d-deform.	1434 C	ia	1434 M	
	ν_5	CH_3 s-deform.	1380 C	ia	1380 W	
	ν_6	CN stretch.	1176 C	ia	1176 VW	
	ν_7	CH_3 rock.	916 C	ia	916 M	
	ν_8	CCN bend.	589 C	ia	589 VS, p	
a_u	ν_9	CH_3 d-stretch.	2966 D	2966 W, sh (solid)	ia	
	ν_{10}	CH_3 d-deform.	1438 C	1438	ia	
	ν_{11}	CH_3 rock.	1109 C	1109 W	ia	
	ν_{12}	CCN bend.	312 D	312 S (solid)	ia	
	ν_{13}	CH_3 torsion	222 D	222 VW	ia	
b_g	ν_{14}	CH_3 d-stretch.	2982 D	ia	2982 VS (solid)	
	ν_{15}	CH_3 d-deform.	1447 D	ia	1447 S (solid)	
	ν_{16}	CH_3 rock.	1010 D	ia	1010 VW	
	ν_{17}	CH_3 torsion	223 D	ia	223 W (solid)	
b_u	ν_{18}	CH_3 d-stretch.	2982 C	2982 VS	ia	
	ν_{19}	CH_3 s-stretch.	2926 C	2926 VS	ia	
	ν_{20}	CH_3 d-deform.	1445 C	1445 S	ia	
	ν_{21}	CH_3 s-deform.	1393 C	1393 M	ia	
	ν_{22}	CN stretch.	1300 C	1300 VW	ia	
	ν_{23}	CH_3 rock.	1009 C	1009 W	ia	
	ν_{24}	CCN bend.	352 C	352 M	ia	

References

[1] IR.R. J. R. Durig, C. B. Pate, and W. C. Harris, J. Chem. Phys. **56**, 5652 (1972).
[2] R.Th. R. A. R. Pearce, I. W. Lewin, and W. C. Harris, J. Chem. Phys. **59**, 1209 (1973).

No. 186 Azomethane-d_6 CD_3NNCD_3
Symmetry C_{2h} **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CD_3 d-stretch.	2227 C	ia	2227 M	
	ν_2	CD_3 s-stretch.	2117 C	ia	2117 S, p	
	ν_3	NN stretch.	1563 C	ia	1563 VW, dp	
	ν_4	CN stretch.	1125 C	ia	1125 W, p	
	ν_5	CD_3 d-deform.	1042 C	ia	1042 M	
	ν_6	CD_3 s-deform.	1035 D	ia	1035 (solid)	
	ν_7	CD_3 rock.	764 C	ia	764 M, p	
	ν_8	CNN bend.	524 C	ia	524 VS, p	
a_u	ν_9	CD_3 d-stretch.	2178 C	2178 VW	ia	
	ν_{10}	CD_3 d-deform.	1043 D	1043 S (solid)	ia	
	ν_{11}	CD_3 rock.	894 D	894 S, b	ia	OV(ν_{23}).
	ν_{12}	CCN bend.	273 C	273 M	ia	
	ν_{13}	CD_3 torsion	166 D	166 VW (solid)	ia	
b_g	ν_{14}	CD_3 d-stretch.	2250 C	ia	2250 M	
	ν_{15}	CD_3 d-deform.	1057 C	ia	1057 M (solid)	
	ν_{16}	CD_3 rock.	792 D	ia	792 W	
	ν_{17}	CD_3 torsion	183 D	ia	183 W (solid)	
b_u	ν_{18}	CD_3 d-stretch.	2239 C	2239 VS	ia	
	ν_{19}	CD_3 s-stretch.	2111 C	2111 M	ia	
	ν_{20}	CN stretch.	1116 D	1116 VW (solid)	ia	
	ν_{21}	CD_3 d-deform.	1047 C	1047 M	ia	
	ν_{22}	CD_3 s-deform.	1029 C	1029 sh	ia	
	ν_{23}	CD_3 rock.	894 D	894 S, b	ia	OV(ν_{11}).
	ν_{24}	CNN bend.	304 C	304 M	ia	

References

See No. 185(CH_3NNCH_3)

No. 187 Carbon suboxide C_3O_2
Symmetry $D_{\infty h}$ **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	CO s-stretch.	2196 B	ia	2196.5 W	
	ν_2	CC s-stretch.	786 B	ia	786.1 W, p	
σ_u^+	ν_3	CO a-stretch.	2258 B	2258 S		
	ν_4	CC a-stretch.	1573 B	1573 S		
π_g	ν_5	CCO bend.	573 C	ia	573.0 W	
π_u	ν_6	CCO bend.	550 B	550 S		
	ν_7	CCC bend,	61 B	61		

References

[1] IR.R. D. A. Long, F. S. Murfin, and R. L. Williams, Proc. Roy. Soc. (London) **A223**, 251 (1984).
[2] IR. F. A. Miller and W. G. Fateley, Spectrochim. Acta **20**, 253 (1964).
[3] IR. W. J. Laffetry, A. G. Maki, and E. K. Plyler, J. Chem. Phys. **40**, 224 (1964).
[4] IR. F. A. Miller, D. H. Lemmon, and R. E. Witowski, Spectrochim. Acta **21**, 1709 (1965).
[5] IR. W. H. Smith and G. E. Leroi, J. Chem. Phys. **45**, 1767 (1966).
[6] Th. R. L. Redington, Spectrochim. Acta **23A**, 1863 (1967).
[7] R. W. H. Smith and J. J. Barrett, J. Chem. Phys. **51**, 1475 (1969).
[8] Th. K. Ramaswarmy and K. Spinivasan, J. Mol. Structure **3**, 473 (1969).
[9] R.IR.Th. L. A. Carreira, R. O. Carter, J. R. Durig, R. C. Lord, and C. C. Milionis, J. Chem. Phys. **59**, 1028 (1973).

No. 188 Carbon subsulfide C_3S_2
Symmetry $D_{\infty h}$ **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (CS_2 soln.)	
σ_g^+	ν_1	CC s-stretch.	1663 D	ia	1663 S	
	ν_2	CS s-stretch.	485 D	ia	485 S, p	
σ_u^+	ν_3	CC a-stretch.	2089 B	2088.5 VS	ia	
	ν_4	CS a-stretch.	1030 B	1029.8 S	ia	
π_g	ν_5	CCS bend.	470 D	ia	470 M	
π_u	ν_6	CCS bend.	502 C	502 VW	ia	
	ν_7	CCC bend.	94 C	94 W	ia	

References

[1] IR.R. W. H. Smith and G. E. Leroi, J. Chem. Phys. **45**, 1778 (1966).
[2] Th. W. H. Smith and G. E. Leroi, J. Chem. Phys. **45**, 1784 (1966).
[3] Th. K. Ramaswarmy and K. Spinivasan, J. Mol. Structure **31**, 473 (1969).

No. 189 Chloro cyanoacetylene ClCCCN

Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (C_6H_6 soln.)	
σ^+	ν_1	CN stretch.	2297 C	2297 VS	2290 VS, p	
	ν_2	C≡C stretch.	2194 B	2194 W	2196 M, p	
	ν_3	C–C stretch.	1093 C	1093 S	1103 W, p	
	ν_4	CCl stretch.	527 B	527 M	530 M, p	
π	ν_5	CCN bend.	483 B	483 S	487 S	
	ν_6	CCC bend.	333 C	333 M	338 M	
	ν_7	CCCl bend.	145 D		145 VW	

References

[1] IR. S. J. Cyvin, E. Kloster–Jensen, and P. Klaboe, Acta Chem. Scand. **19**, 903 (1965).
[2] IR.R. P. Klaboe and E. Kloster–Jensen, Spectrochim. Acta **23A**, 1981 (1967).

No. 190 Bromo cyanoacetylene BrCCCN

Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (C_6H_6 soln.)	
σ^+	ν_1	CN stretch.	2292 C	2292 VS	2276 VS, p	
	ν_2	C≡C stretch.	2150 C	2150 S	2123 W	
	ν_3	C–C stretch.	1054 B	1054 VW	1052 W	
	ν_4	CBr stretch.	419 B	419 W	418 M, p	
π	ν_5	CCN bend.	485 B	485 S	489 S	
	ν_6	CCC bend.	312 B	312 M	317 S	
	ν_7	CCBr bend.	142 D		142 VW	

References

See No. 189(ClCCCN).

No. 191 Iodo cyanoacetylene ICCCN
Symmetry $C_{\infty v}$ Symmetry number σ = 1

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (C_6H_6 soln.)	
σ^+	ν_1	CN stretch.	2270 C	2270 S	2265 VS, p	
	ν_2	C≡C stretch.	2131 C	2131 M	2125 M, p	
	ν_3	C–C stretch.	1031 C	1031 S	1034 W, p	
	ν_4	CI stretch.	364 B	364 W	356 M	
π	ν_5	CCN bend.	496 B	496 M	497 S, dp	
	ν_6	CCC bend.	309 C	309 W	315 M, dp	
	ν_7	CCI bend.	130 D		130 VW	

References
See No. 189(ClCCCN).

No. 192 Chloropropadiene CH_2CCHCl
Symmetry C_s Symmetry number σ = 1

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH stretch.	3079 C	3079 S	3062 S, p	OV(ν_{11}).
	ν_2	CH_2 s–stretch.	3009 C	3009 M	2990 S, p	
	ν_3	CCC a–stretch.	1963 C	1963 M	1951 W, dp	
	ν_4	CH_2 scis.	1435 C	1435 S	1419 S, p	
	ν_5	CH bend.	1256 C	1256 VS	1244 W, p	
	ν_6	CCC s–stretch.	1101 C	1101 S	1095 VS, p	
	ν_7	CH_2 wag.	875 C	875 VS	877 W, dp	
	ν_8	CCl stretch.	767 C	767 VS	751 W, dp	
	ν_9	CCC deform.	592 C	592 W		
	ν_{10}	CCCl deform.	494 C	494 M	490 VS, p	
a''	ν_{11}	CH_2 a–stretch.	3079 C	3079 S	3062 S, p	OV(ν_1).
	ν_{12}	CH_2 rock.	999 B	999 W	995 W, dp	
	ν_{13}	CH bend.	822 B	822 S	815 W, dp	
	ν_{14}	CCC deform.	548 B	548 M	546 W, dp	
	ν_{15}	CCCl deform.	184 C		184 S, dp	

Reference
[1] IR.R. R. A. Nyquist, Y. S. Lo, and J. C. Evans, Spectrochim. Acta **20**, 619 (1964).

No. 193 Bromopropadiene CH_2CCHBr
Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH stretch.	3080 C	3080 M	3060 (46), p	OV(ν_{11}).
	ν_2	CH_2 s-stretch.	3005 C	3005 M	2985 (63), p	
	ν_3	CCC a-stretch.	1961 C	1961 W	1954 (19), p	
	ν_4	CH_2 scis.	1432 B	1432 S	1422	
	ν_5	CH bend.	1217 C	1217 VS	1209 (12)	
	ν_6	CCC s-stretch.	1078 C	1078 W	1086 (29), p	
	ν_7	CH_2 wag.	862 C	862 VS	873 (3), dp	
	ν_8	CBr stretch.	681 C	681 VS	667 (31), p	
	ν_9	CCC deform.	603 C	603 W		
	ν_{10}	CCBr deform.	423 C	423 VW (CS_2 soln.)	426 (33), p	
a''	ν_{11}	CH_2 a-stretch.	3080 C	3080 M	3060 (46), p	OV(ν_1).
	ν_{12}	CH_2 rock.	1000 B	1000 W		
	ν_{13}	CH bend.	812 B	812 S	806 (3), dp	
	ν_{14}	CCC deform.	519 B	519 M		
	ν_{15}	CCCl deform.	169 C		169 (43b), dp	

Reference
See No. 192(CH_2CCHCl).

No. 194 Iodopropadiene CH_2CCHI
Symmetry C_s **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH stretch.	3070 C	3070 M	3057 M	OV(ν_{11}).
	ν_3	CCC a-stretch.	1953 C	1953 M	1947 VS	
	ν_2	CH_2 s-stretch.	3004 C	3004 W	2978 VS	
	ν_4	CH_2 scis.	1425 B	1425 M	1412 VS	
	ν_5	CH bend.	1178 C	1178 VS	1174 S, p	
	ν_6	CCC s-stretch.	1076 C	1076 M	1076 VS, p	
	ν_7	CH_2 wag.	854 C	854 S		
	ν_8	CCC deform.	625 C	625 S	635 W	
	ν_9	CI stretch.	609 C	609 S		
	ν_{10}	CCI drform.	387 C		387 S, p	
a''	ν_{11}	CH_2 a-stretch.	3070 C	3070 M	3057 M	OV(ν_1).
	ν_{12}	CH_2 rock.	995 B	995 W		
	ν_{13}	CH bend.	807 B	807 S		
	ν_{14}	CCC deform.	485 B	485 W		
	ν_{15}	CCI deform.	154 C		154 W	

Reference
See No. 192(CH_2CCHCl).

No. 195 Trifluoropropyne CF_3CCH
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch.	3327 B	3327.3 S	3316 (9) p	
	ν_2	C≡C stretch.	2165 C	2165.4 S	2156 (80) p	FR($\nu_4+\nu_6+\nu_{10}$).
	ν_3	CF_3 s-stretch.	1253 B	1253.2 VS	1250 (1b)	
	ν_4	C–C stretch.	812 B	811.9 W	810 (50) p	
	ν_5	CF_3 s-deform.	536 B	536.1 M	537 (11) p	
e	ν_6	CF_3 d-stretch.	1179 B	1179.2 VS	1155 (5b) dp	
	ν_7	CH bend.	686 B	685.5 S	696 (6) dp	
	ν_8	CF_3 d-deform.	612 B	611.9 M	606 (4) dp	
	ν_9	CF_3 rock.	453 B	453.0 M	445 (6) dp	
	ν_{10}	CCC bend.	171 B	171 M	170 (100) dp	

References

[1] IR.R. C. V. Berney, L. R. Cousins, and F. A. Miller, Spectrochim. Acta **19**, 2019 (1963).
[2] IR. R. H. Sanborn, Spectrochim. Acta **23A**, 1999 (1967).

No. 196 Trifluoropropyne–d CF_3CCD
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD stretch.	2626 B	2626.0 M		
	ν_2	C≡C stretch.	2014 B	2013.9 S		
	ν_3	CF_3 s-stretch.	1250 B	1249.7 VS		
	ν_4	C–C stretch.	808 B	808.4 W		
	ν_5	CF_3 s-deform.	529 B	528.9 M		
e	ν_6	CF_3 d-stretch.	1179 B	1179.0 VS		
	ν_8	CF_3 d-deform.	611 B	611.3 M		
	ν_7	CD bend.	539 B	538.5 S		
	ν_9	CF_3 rock.	456 B	455.5 M		
	ν_{10}	CCC bend.	163 B	163 M		

References

[1] IR.R. C. V. Berney, L. R. Cousins, and F. A. Miller, Spectrochim. Acta **19**, 2019 (1963).
[2] IR. R. H. Sanborn, Spectrochim. Acta **23A**, 1999 (1967).

No. 197 1-Chloro-3,3,3-trifluoropropyne CF_3CCCl
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	C≡C stretch.	2270 C	2270 VS	2266 S, p	
	ν_2	CF_3 s-stretch.	1276 C	1276 VS	1272 W	
	ν_3	C-C stretch.	937 C	937 S	933 S, p	
	ν_4	CCl stretch.	723 C	723 S	723 S, p	
	ν_5	CF_3 s-deform.	377 C	377 W	374 S, p	
e	ν_6	CF_3 d-stretch.	1174 C	1174 VS	1153 W, b	
	ν_7	CF_3 d-deform.	606 C	606 M	603 W	
	ν_8	CF_3 rock.	448 D		448 M, dp	
	ν_9	CCCCl deform.	311 C	311 W	316 VS, dp	
	ν_{10}	CCCCl deform.	97 D		97 VS, dp	

Reference

[1] IR.R. E. Augdahl, E. Kloster-Jensen, V. Devarajan and S. J. Cyvin, Spectrochim. Acta **29A**, 1329 (1973).

No. 198 1-Bromo-3,3,3-trifluoropropyne CF_3CCBr
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	C≡C stretch.	2243 C	2243 S	2236 M, p	
	ν_2	CF_3 s-stretch.	1275 C	1275 VS	1267 W	
	ν_3	C-C stretch.	883 C	883 S	879 S, p	
	ν_4	CBr stretch.	687 C	687 S	684 M, p	
	ν_5	CF_3 s-deform.	285 D	285 M	292 VS	
e	ν_6	CF_3 d-stretch.	1176 C	1176 VS	1155 W, b	
	ν_7	CF_3 d-deform.	607 C	607 M	606 W	
	ν_8	CF_3 rock.	455 D	455 VW	452 S	
	ν_9	CCCBr deform.	278 D	278 VW, sh		
	ν_{10}	CCCBr deform.	90 D		90 VS, dp	

Reference

See No. 197(CF_3CCCl).

No. 199 1-Iodo-3,3,3-trifluoropropyne CF_3CCI
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	C≡C stretch.	2218 C	2218 S	2207 S, p	
	ν_2	CF_3 s-stretch.	1264 C	1264 VS	1253 W	
	ν_3	C–C stretch.	857 C	857 M	857 S, p	
	ν_4	CI stretch.	661 C	661 S	658 M	
	ν_5	CF_3 s-deform.	250 D	250 W, sh	254 VS, p	
e	ν_6	CF_3 d-stretch.	1174 C	1174 VS	1150 W, b	
	ν_7	CF_3 d-deform.	608 C	608 W	605 W	
	ν_8	CF_3 rock.	450 C	450 W	449 M, dp	
	ν_9	CCCI deform.	263 C	263 M	267 VS, dp	
	ν_{10}	CCCI deform.	85 D		85 VS, dp	

Reference
See No. 197(CF_3CCCl).

No. 200 Propargyl fluoride $CHCCH_2F$
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH stretch.	3338 C	3338 S	3330 (4), p	
	ν_2	CH_2 s-stretch.	2955 C	2955 M	2960 (22), p	
	ν_3	C=C stretch.	2150 C	2150 W	2135 (43), p	
	ν_4	CH_2 scis.	1465 C	1465 VW	1458 (3), dp	
	ν_5	CH_2 wag.	1381 C	1381 S	1374 (3), dp	
	ν_6	CF stretch.	1039 C	1039 VS		
	ν_7	C–C stretch.	940 C	940 M	935 (6), p	
	ν_8	CH bend.	675 C	675 S (CS_2 soln.)	692 (1), dp	
	ν_9	CCF deform.	539 C	539 W	544 (3), p	
	ν_{10}	CCC deform.	211 C		211 (10), dp	
a''	ν_{11}	CH_2 a-stretch.	2972 C	2972 M	2986 (7), dp	
	ν_{12}	CH_2 twist.	1242 D	1240 VW	1242 (1), dp	
	ν_{13}	CH_2 rock.	1018 D	1018 W	1012 (3b), p	
	ν_{14}	CH bend.	635 C	635 S	646 (1b), dp	
	ν_{15}	CCC deform.	310 C		310 (4), dp	

Reference
[1] IR.R. J. C. Evans and R. A. Nyquist, Spectrochim. Acta **19**, 1153 (1963).

No. 201 Propargyl chloride $CHCCH_2Cl$
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a'	ν_1	CH stretch.	3335 C	3335 VS	3305 (2), p	
	ν_2	CH_2 s-stretch.	2968 C	2968 M	2957 (29), p	
	ν_3	C≡C stretch.	2147 C	2147 W	2130 (35), p	
	ν_4	CH_2 scis.	1441 C	1441 M	1432 (2), p	
	ν_5	CH_2 wag.	1271 C	1271 VS	1267 (5), p	
	ν_6	C–C stretch.	960 C	960 S	961 (2), dp	
	ν_7	CCl stretch.	725 C	725 VS	713 (12), p	
	ν_8	CH bend.	650 D	650 S (CS_2 soln.)	650 (2b)	
	ν_9	CCCl deform.	451 C	451	452 (5), p	
	ν_{10}	CCC deform.	186 D		186 (10), dp	
a''	ν_{11}	CH_2 a-stretch.	3002 C	3002 M	2995 (4), dp	
	ν_{12}	CH_2 twist.	1179 B	1179 W	1174 (1), dp	
	ν_{13}	CH_2 rock.	908 D		908 (1), dp	
	ν_{14}	CH bend.	637 D	637 M	650 (2b), dp	
	ν_{15}	CCC deform.	311 C		311 (4), dp	

Reference
See No. 200($CHCCH_2F$).

No. 202 Propargyl bromide $CHCCH_2Br$
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a'	ν_1	CH stretch.	3335 C	3335 S	3305 (2), p	
	ν_2	CH_2 s-stretch.	2976 C	2976 W	2958 (20), p	
	ν_3	C≡C stretch.	2138 D	2138 VW	2125 (36), p	
	ν_4	CH_2 scis.	1431 C	1431 W	1425 (2), dp	
	ν_5	CH_2 wag.	1218 C	1218 S	1214 (9), p	
	ν_6	C–C stretch.	961 C	961 M	962 (3), p	
	ν_7	CH bend.	652 C	652 VS (CS_2 soln.)		
	ν_8	CBr stretch.	621 C	621 S	618 (22), p	
	ν_9	CCBr deform.	399 C	399 (CS_2 soln.) (soln.)	399 (9), p	
	ν_{10}	CCC deform.	168 C		168 (10), p	
a''	ν_{11}	CH_2 a-stretch.	3006 C	3006 (CS_2 soln.)	3008 (4), p	
	ν_{12}	CH_2 twist.	1152 D	1152 VW	1146 (1)	
	ν_{13}	CH_2 rock.	866 D		866 (1), dp	
	ν_{14}	CH bend.	637 C	637 S		
	ν_{15}	CCC deform.	314 C		314 (3), dp	

Reference
See No. 200($CHCCH_2F$).

No. 203 Propargyl iodide $CHCCH_2I$
Symmetry C_s **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency cm^{-1}	Infrared cm^{-1}	Raman cm^{-1}	Comments
				(Gas)	(Liquid)	
a'	ν_1	CH stretch.	3335 C	3335 S		
	ν_2	CH_2 s-stretch.	2958 C	2958 (CS_2 soln.)	2957 VS	
	ν_3	C≡C stretch.	2130 C	2130 C (CCl_4 soln.)	2128 VS	
	ν_4	CH_2 scis.	1423 C	1423 W	1414	
	ν_5	CH_2 wag.	1160 C	1160 M	1160 VS	
	ν_6	C–C stretch.	959 C	959 W	964 S	
	ν_7	CH bend.	640 C	640 S	650 VW,b	OV(ν_{14}).
	ν_8	CI stretch.	570 C	570 W	567 VS	
	ν_9	CCI deform.	364 C		364 S	
	ν_{10}	CCC deform.	157 C		157 M	
a''	ν_{11}	CH_2 a-stretch.	3008 D	3008 (CS_2 soln.)	2990 b	
	ν_{12}	CH_2 twist.	1116 D	1116 (CS_2 soln.)		
	ν_{13}	CH_2 rock.	810 E[a]			
	ν_{14}	CH bend.	640 D	640 S	650 VW, b	OV(ν_7).
	ν_{15}	CCC deform.	314 C		314 VW	

[a] Estimated from the corresponding frequencies of other propargyl halides.

Reference

See No. 200($CHCCH_2F$).

No. 204 Chlorodiacetylene ClCCCCH
Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency cm^{-1}	Infrared cm^{-1}	Raman cm^{-1}	Comments
				(Gas)		
σ^+	ν_1	CH stretch.	3327 C	3327 VS		
	ν_2	C≡C a-stretch.	2252 C	2252 VS		
	ν_3	C≡C s-stretch.	2071 C	2071 M		
	ν_4	C–C stretch.	1093 C	1093 S		
	ν_5	CCl stretch.	525 C	525 S		
π	ν_6	CH bend.	621 B	621 VS		
	ν_7	CCCC a-bend.	463 B	463 S		
	ν_8	CCCC s-bend.	335 C	335 M		
	ν_9	CCCl bend.	133 E	133		OC($\nu_7+\nu_9$, $\nu_6+\nu_9$, $\nu_7+\nu_9$).

Reference

[1] IR. P. Klaboe and E. Kloster-Jensen, Spectrochim. Acta **23A**, 2733 (1967).

No. 205 Bromodiacetylene BrCCCCH
Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	CH stretch.	3335 C	3335 VS		
	ν_2	C≡C a-stretch.	2237 C	2237 S		
	ν_3	C≡C s-stretch.	2095 C	2095 W		
	ν_4	C–C stretch.	1046 C	1046 M		
	ν_5	CBr stretch.	425 C	425 M		
π	ν_6	CH bend.	623 C	623 VS		
	ν_7	CCCC a-bend.	470 B	470 S		
	ν_8	CCCC s-bend.	355 B	355 M		
	ν_9	CCBr bend.	118 E			OC($\nu_1+\nu_9$, $\nu_7+\nu_9$).

Reference
See No. 204(ClCCCH).

No. 206 Iododiacetylene ICCCCH
Symmetry $C_{\infty v}$ **Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
σ^-	ν_1	CH stretch.	3332 C	3332 VS		
	ν_2	C≡C a-stretch.	2211 C	2211 S		
	ν_3	C≡C s-stretch.	2060 C	2060 VW		
	ν_4	C–C stretch.	1025 D	1025 VW (CS_2 soln.)		
	ν_5	CI stretch.	362 C	362 M		
π	ν_6	CH bend.	623 B	623 VS		
	ν_7	CCCC a-bend.	473 B	473 M		
	ν_8	CCCC s-bend.	357 C	357 W		
	ν_9	CCI bend.	110 E	110		OC($\nu_8+\nu_9$,$\nu_7+\nu_9$).

Reference
See No. 204(ClCCCH).

No. 207 1,4-Dioxane $C_4H_8O_2$
Symmetry C_{2h} ***Symmetry number σ = 2***

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CH_2 a-stretch.	2968 C	ia	2968 S, p	
	ν_2	CH_2 s-stretch.	2856 C	ia	2856 S, p	
	ν_3	CH_2 scis.	1444 C	ia	1444 M, p	
	ν_4	CH_2 wag.	1397 C	ia	1397 W, p	
	ν_5	CH_2 twist.	1305 C	ia	1305 S, p	
	ν_6	CH_2 rock.	1128 C	ia	1128 M, p	
	ν_7	CC stretch.	1015 C	ia	1015 S, p	
	ν_8	CO stretch.	837 C	ia	837 VS, p	
	ν_9	OCC deform.	435 C	ia	435 M	
	ν_{10}	COC deform.	424 C	ia	424 M, p	
a_u	ν_{11}	CH_2 a-stretch.	2970 C	2970 M	ia	
	ν_{12}	CH_2 s-stretch.	2863 C	2863 VS	ia	
	ν_{13}	CH_2 scis.	1449 C	1449 S	ia	
	ν_{14}	CH_2 wag.	1369 C	1369 S	ia	
	ν_{15}	CH_2 twist.	1256 C	1256 S	ia	
	ν_{16}	CO stretch.	1136 C	1136 VS	ia	
	ν_{17}	CH_2 rock.	1086 C	1086 S	ia	
	ν_{18}	CC stretch.	881 C	881 S	ia	
	ν_{19}	OCC deform.	288 C	288 W,sh	ia	
b_g	ν_{20}	CH_2 a-stretch.	2968 C	ia	2968 S, p	SF(ν_1).
	ν_{21}	CH_2 s-stretch.	2856 C	ia	2856 S, p	SF(ν_2).
	ν_{22}	CH_2 scis.	1459 C	ia	1459 M, dp	
	ν_{23}	CH_2 wag.	1335 C	ia	1335 W	
	ν_{24}	CH_2 twist.	1217 C	ia	1217 M, dp	
	ν_{25}	CO stretch.	1110 C	ia	1110 M, dp	
	ν_{26}	CH_2 rock.	853 C	ia	853 M,sh, dp	
	ν_{27}	OCC deform.	490 C	ia	490 M, dp	
b_u	ν_{28}	CH_2 a-stretch.	2970 C	2970 M	ia	SF(ν_{11}).
	ν_{29}	CH_2 a-stretch.	2863 C	2863 VS	ia	SF(ν_{12}).
	ν_{30}	CH_2 scis.	1457 C	1457 S	ia	
	ν_{31}	CH_2 wag.	1378 C	1378 M	ia	
	ν_{32}	CH_2 twist.	1291 C	1291 S	ia	
	ν_{33}	CH_2 rock.	1052 C	1052 S	ia	
	ν_{34}	CO stretch.	889 C	889 S	ia	
	ν_{35}	OCC deform.	610 C	610 S	ia	
	ν_{36}	COC deform.	274 C	274 S	ia	

References

[1] IR.R. F. E. Malherbe and H. J. Bernstein, J. Amer. Chem. Soc. **74**, 4408 (1952), and references cited there.
[2] IR.Th. R. G. Snyder and G. Zerbi, Spectrochim. Acta **23A**, 391 (1967).
[3] IR.R.Th. O. H. Ellested and P. Klaboe, Spectrochim. Acta **27A**, 1025 (1971).

No. 208 Diethynyl ketone $(HC\equiv C)_2CO$
Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (Liquid)	
a_1	ν_1	CH stretch.	3325 C	3325 S	3275 W, b	OV(ν_{13}).
	ν_2	C≡C stretch.	2097 C	2098 VS, sh (liquid)	2097 VS, p	
	ν_3	CO stretch.	1669 C	1669 S	1636 S, p	
	ν_4	C–C stretch.	739 C	739 VW	749 M, p	
	ν_5	CH bend.	648 C	648 S		
	ν_6	C–C–C deform.	571 C		571 W	
	ν_7	C≡C–C deform.	122 C	122 VW		
a_2	ν_8	CH bend.	712 C	ia	712 VW, dp	
	ν_9	C≡C–C deform.	268 C	ia	268 M	
b_1	ν_{10}	CH bend.	729 C	729 S	733 VW (solid)	
	ν_{11}	CO op–bend.	688 C	688 S	689 VW	
	ν_{12}	C≡C–C deform.	190 C	190 VW	200 W	
b_2	ν_{13}	CH stretch.	3325 C	3325 S	3275 VW, b	OV(ν_1).
	ν_{14}	C≡C stretch.	2115 C	2115 S	2107 M	
	ν_{15}	C–C stretch.	1144 C	1144 VS		
	ν_{16}	CH bend.	682 C	682 M		
	ν_{17}	CO ip–bend.	548 C	548 M		
	ν_{18}	C≡C–C deform.	229 C	229 VW	239 M	

Reference

[1] IR.R. F. A. Miller, B. M. Harney, and J. Tyrrell, Spectrochim. Acta **27A**, 1003 (1971).

No. 209 Dicyanodiacetylene NCCCCCCN
Symmetry $D_{\infty h}$ **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm⁻¹	cm⁻¹ (Gas)	cm⁻¹ (CCl_4 soln.)	
σ_g^+	ν_1	CN s–stretch.	2235 C	ia	2235 VS, p	
	ν_2	C≡C s–stretch.	2183 C	ia	2183 M, p	
	ν_3	C–C s–stretch.	1288 C	ia	1287.5 W, p	
	ν_4	C–C stretch.	571	ia	571 W, dp	
σ_u^+	ν_5	CN a–stretch.	2266 B	2266 S	ia	
	ν_6	C≡C a–stretch.	2097 B	2097 M	ia	
	ν_7	C–C a–stretch.	717 B	717 S	ia	
π_g	ν_8	Bend.	501 C	ia	501 M, dp	
	ν_9	Bend.	455 C	ia	455 W, dp (C_6H_{14} soln.)	
	ν_{10}	Bend.	170 D	ia	170 W, b, dp	
π_u	ν_{11}	Bend.	491 B	490.5 VS	ia	
	ν_{12}	Bend.	276 B	276 VS	ia	
	ν_{13}	Bend.	62 B	61.5 VS	ia	

Reference

[1] IR.R. F. A. Miller and D. H. Lemmon, Spectrochim. Acta **23A**, 1415 (1967).

No. 210 Hexacarbonylchromium(0) $Cr(^{12}C^{16}O)_6$
Symmetry O_h **Symmetry number σ = 24**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (CCl_4 soln.)	
a_{1g}	ν_1	CO stretch.	2112 C	ia	2112.4 M	
	ν_2	CrC stretch.	381 C	ia	381.2 S	
e_g	ν_3	CO stretch.	2018 C	ia	2018.4 M	
	ν_4	CrC stretch.	394 D	ia	394 W	
f_{1g}	ν_5	CrCO bend.	364 D	ia	ia	OC($\nu_5+\nu_7$).
f_{1u}	ν_6	CO stretch.	2000 B	2000.4 VS	ia	
	ν_7	CrC stretch.	668 B	668.1 VS	ia	
	ν_8	CrCO bend.	441 B	440.5 S	ia	
	ν_9	CCrC deform.	98 B	97.8 M	ia	
f_{2g}	ν_{10}	CrCO bend.	436 D	ia	436.4 (liquid)	
	ν_{11}	CCrC deform.	95 D	ia	94.8 S (liquid)	
f_{2u}	ν_{12}	CrCO bend.	511 D	ia	ia	OC($\nu_{10}+\nu_{12}$, $\nu_5+\nu_{12}$).
	ν_{13}	CCrC deform.	68 E	ia	ia	OC($\nu_3+\nu_{13}$).

References

[1] IR. N. J. Hawkins, H. C. Mattraw, W. W. Sabol, and D. R. Carpenter, J. Chem. Phys. **23**, 2422 (1955).
[2] Th. H. Murata and K. Kawai, J. Chem. Phys. **27**, 605 (1957).
[3] IR.Th. L. H. Jones, Spectrochim. Acta **19**, 329 (1963).
[4] IR.Th. J. M. Smith and L. H. Jones, J. Mol. Spectry. **20**, 248 (1966).
[5] IR.R.Th. L. H. Jones, R. S. McDowell, and M. Goldblatt, Inorg. Chem. **8**, 2349 (1969).
[6] R.Th. R. Pince et R. Poilblanc, Spectrochim. Acta **28A**, 907 (1972).

No. 211 Hexacarbonylmolybdenum(0) $Mo(^{12}C^{16}O)_6$
Symmetry O_h Symmetry number σ = 24

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (CCl_4 soln.)	
a_{1g}	ν_1	CO stretch.	2117 C	ia	2116.7 M	
	ν_2	MoC stretch.	402 C	ia	402.2 S	
e_g	ν_3	CO stretch.	2019 C	ia	2018.8 M	
	ν_4	MoC stretch.	392 C	ia	392 W	
f_{1g}	ν_5	MoCO bend.	342 D	ia	ia	OC($\nu_5+\nu_7$).
f_{1u}	ν_6	CO stretch.	2003 B	2003.0 VS	ia	
	ν_7	MoC stretch.	596 B	595.6 VS	ia	
	ν_8	MoCO bend.	367 B	367.2 S	ia	
	ν_9	CMoC deform.	82 B	81.6 M	ia	
f_{2g}	ν_{10}	MoCO bend.	448 D	ia	448.3 (liquid)	
	ν_{11}	CMoC deform.	86 D	ia	86.0 S (liquid)	
f_{2u}	ν_{12}	MoCO bend.	507 D	ia	ia	OC($\nu_5+\nu_{12}$, $\nu_{10}+\nu_{12}$)
	ν_{13}	CMoC deform.	60 E	ia	ia	OC($\nu_3+\nu_{13}$, $\nu_{10}+\nu_{13}$).

References

[1] IR. N. J. Hawkins, H. C. Mattraw, W. W. Sabol, and D. R. Carpenter, J. Chem. Phys. **23**, 2422 (1955).
[2] Th. H. Murata and K. Kawai, J. Chem. Phys. **27**, 605 (1957).
[3] IR. L. H. Jones, J. Chem. Phys. **36**, 2375 (1962).
[4] IR.Th. L. H. Jones, Spectrochim. Acta **19**, 329 (1963).
[5] IR.Th. J. M. Smith and L. H. Jones, J. Mol. Spectry. **20**, 248 (1966).
[6] IR.R.Th. L. H. Jones, R. S. McDowell, and M. Goldblatt, Inorg. Chem. **8**, 2349 (1969).
[7] R.Th. R. Pince et R. Poilblanc, Spectrochim. Acta **28A**, 907 (1972).

No. 212 Hexacarbonyltungsten(0) $W(^{12}C^{16}O)_6$
Symmetry O_h **Symmetry number $\sigma = 24$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (CS_2 soln.)	
a_{1g}	ν_1	CO stretch.	2117 C	ia	2116.6 M	
	ν_2	WC stretch.	427 C	ia	427.1 S	
e_g	ν_3	CO stretch.	2010 C	ia	2009.8 M	
	ν_4	WC stretch.	412 C	ia	412 W	
f_{1g}	ν_5	WCO bend.	362 D	ia	ia	OC($\nu_5+\nu_7$).
f_{1u}	ν_6	CO stretch.	1998 B	1997.6 VS	ia	
	ν_7	WC stretch.	587 B	586.6 VS	ia	
	ν_8	WCO bend.	374 B	374.4 S	ia	
	ν_9	CWC deform.	82 C	82.0 M	ia	
f_{2g}	ν_{10}	WCO bend.	458 D	ia	458.3 (liquid)	
	ν_{11}	CWC deform.	88 D	ia	88.3 S (liquid)	
f_{2u}	ν_{12}	WCO bend.	521 D	ia	ia	OC($\nu_5+\nu_7$, $\nu_{10}+\nu_{12}$).
	ν_{13}	CWC deform.	61 E	ia	ia	OC($\nu_3+\nu_{13}$).

References

[1] IR.Th. L. H. Jones, Spectrochim. Acta **19**, 329 (1963).
[2] IR.Th. J. M. Smith and L. H. Jones, J. Mol. Spectry. **20**, 248 (1966).
[3] IR.R.Th. L. H. Jones, R. S. McDowell, and M. Goldblatt, Inorg. Chem. **8**, 2349 (1969).
[4] R.Th. R. Pince et R. Poilblanc, Spectrochim. Acta **28A**, 907 (1972).

Empirical Formula Index for Consolidated Volumes I and II

In this index molecules are divided into two groups: (a) those containing no carbon atoms, which are arranged with the elemental symbols of the empirical formulas in alphabetical order and are listed alphabetically, and in ascending order of the empirical formula subscripts; (b) molecules containing carbon, which are ordered in the same way except that carbon is listed first and hydrogen second. No distinction is made for isotopic species in the empirical formula; thus deuterium is listed as H.

As an assistance to users of these data, this Index identifies the molecules treated in the present Consolidated Volume II and also those in the earlier Consolidated Volume I, which is available as part of a previous publication series, the NSRDS-NBS series distributed by the U.S. Government Printing Office. It can be ordered as Tables of Molecular Vibrational Frequencies, Consolidated Volume I, (SD Catalog No. C13.48:39), stock number 003-003-00845-1, price $5.10, from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

Compounds Not Containing Carbon

Empirical Formula	Name	Volume and Number
$AlCl_3$	Aluminum trichloride	II–36
AsF_3	Arsenic trifluoride	II–38
AsF_5	Arsenic pentafluoride	II–118
AsH_3	Arsine	I–21
AsH_3	Arsine–d_3	I–22
AsI_3	Arsenic triodide	II–39
BF_3	Boron trifluoride–$^{10}BF_3$	II–31
BF_3	Boron trifluoride–$^{11}BF_3$	II–22
B_2H_6	Diborane–$^{10}B_2H_6$	I–55
B_2H_6	Diborane–$^{11}B_2D_6$	I–56
$BrCl_3Si$	Bromotrichlorosilane	I–45
BrF_3	Bromine trifluoride	II–46
$BrGeH_3$	Germyl bromide	II–88
$BrGeH_3$	Germyl bromide–d_3	II–89
BrH_3Si	Silyl bromide	I–44
BrNO	Nitrosyl bromide–$^{16}O^{14}NBr$	II–23
BrNO	Nitrosyl bromide–$^{16}O^{15}NBr$	II–24
BrNO	Nitrosyl bromide–$^{18}O^{15}NBr$	II–25
BrO_3Re	Rhenium (VII) oxide bromide	II–95
Br_2Cl_2Si	Dibromodichlorosilane	I–49
Br_2FOP	Phosphoryl dibromofluoride	II–111
Br_2H_2Si	Dibromosilane	II–100
Br_2OS	Thionyl bromide	II–57
Br_2Sn	Tin (II) bromide	II–12

Empirical Formula	Name	Volume and Number
Br_3ClSi	Tribromochlorosilane	I–47
Br_3GeH	Tribromogermane	II–93
Br_3HSi	Tribromosilane	II–75
Br_3OP	Phosphoryl bromide	II–78
Br_4Ge	Germanium tetrabromide	I–39
Br_4Hf	Hafnium tetrabromide	II–66
Br_4Si	Silicon tetrabromide	I–31
Br_4Sn	Tin (IV) bromide	I–41
Br_4Ti	Titanium tetrabromide	II–59
Br_4Zn	Zirconium tetrabromide	II–62
$ClFO_3$	Perchloryl fluoride	II 81
ClF_2N	Chlorodifluoroammonia	II–53
ClF_2PS	Thiophosphoryl chlorodifluoride	II–112
ClF_3	Chlorine trifluoride	II–45
ClF_5S	Sulfur chloride pentafluoride	II–122
ClF_5W	Tungsten chloride pentafluoride	II–123
$ClGeH_3$	Germyl chloride	II–86
$ClGeH_3$–d_3	Germyl chloride–d_3	II–87
ClHO	Hypochlorous acid	II–27
ClHO	Hypochlorous acid–d	II–28
ClH_3Si	Silyl chloride	I–43
ClI_3Si	Chlorotriiodosilane	I–48
ClNO	Nitrosyl chloride–$^{16}O^{14}NO$	II–19
ClNO	Nitrosyl chloride–$^{16}O^{15}NCl$	II–20
ClNO	Nitrosyl chloride–$^{18}O^{14}NCl$	II–21
ClNO	Nitrosyl chloride–$^{18}O^{15}NCl$	II–22
$ClNO_2$	Nitryl chloride-$Cl^{14}NO_2$	II–43
$ClNO_2$	Nitryl chloride-$Cl^{15}NO_2$	II–44
$ClNO_3$	Chloronitrate-$ClO^{14}NO_2$	II–108
$ClNO_3$	Chloronitrate-$ClO^{15}NO_2$	II–109
ClNS	Thionitrosyl–S–chloride	II–30
ClO_3Re	Rhenium (VII) oxide chloride	II–94
Cl_2FN	Dichlorofluoroammonia	II–54
Cl_2FOP	Phosphoryl dichlorofluoride	II–110
Cl_2FPS	Thiophosphoryl dichlorofluoride	II–113
Cl_2Ge	Germanium (II) chloride	II–9
Cl_2H_2Si	Dichlorosilane	II–98
Cl_2H_2Si	Dichlorosilane–d_2	II 99
Cl_2O	Oxygen dichloride	I–8
Cl_2OS	Thionyl chloride	II–56
Cl_2O_2S	Sulfuryl chloride	II–97
Cl_2Pb	Lead (II) chloride	II–14
Cl_2S	Sulfur dichloride	II–8
Cl_2Sn	Tin (II) chloride	II–11
Cl_3F_2P	Phosphorus trichloride difluoride	II–115
Cl_3GeH	Trichlorogermane	II–92
Cl_3HSi	Trichlorosilane	II–73
Cl_3HSi	Trichlorosilane–d	II–74
Cl_3ISi	Trichloroiodosilane	I–46
Cl_3OP	Phosphoryl chloride	II–77
Cl_3OV	Vanadyl (V) chloride	II–82

Empirical Formula	Name	Volume and Number
Cl_3P	Phosphorus trichloride	I–20
Cl_3PS	Thiophosphoryl trichloride	II–80
Cl_4Ge	Germanium tetrachloride	I–38
Cl_4Hf	Hafnium tetrachloride	II–65
Cl_4Si	Silicon tetrachloride	I–30
Cl_4Sn	Tin (IV) chloride	I–40
Cl_4Ti	Titanium tetrachloride	II–58
Cl_4Zn	Zirconium tetrachloride	II–61
Cl_5P	Phosphorus pentachloride	II–116
Cl_5Sb	Antimony pentachloride	II–119
$FGeH_3$	Germyl fluoride	II–84
$FGeH_3$	Germyl fluoride–d_3	II–85
FHO	Hypofluorous acid	II–26
FH_3Si	Silyl fluoride	I–42
$FMnO_3$	Permanganyl fluoride	II–83
FNO	Nitrosyl fluoride–$^{16}O^{14}NF$	II–15
FNO	Nitrosyl fluoride–$^{16}O^{15}NF$	II–16
FNO	Nitrosyl fluoride–$^{18}O^{14}NF$	II–17
FNO	Nitrosyl fluoride–$^{18}O^{15}NF$	II–18
FNO_2	Nitryl fluoride–$F^{14}NO_2$	II–41
FNO_2	Nitryl fluoride–$F^{15}NO_2$	II–42
FNO_3	Fluoronitrate-$FO^{14}NO_2$	II–106
FNO_3	Fluoronitrate-$FO^{15}NO_2$	II–107
FNS	Thionitrosyl–S–fluoride	II–29
F_2HN	Difluoroamine	II–52
F_2N_2	trans–1,2–Difluorodiazine	II–40
F_2O	Oxygen difluoride	I–7
F_2Kr	Krypton difluoride	II–1
F_2OS	Thionyl fluoride	II–55
F_2O_2S	Sulfuryl fluoride	II–96
F_2O_2Se	Selenium dioxide difluoride	II–101
F_2Pb	Lead (II) fluoride	II–13
F_2S_2	Difluoro disulfane	II–49
F_2Sn	Tin (II) fluoride	II–10
F_3HSi	Trifluorosilane	II–71
F_3HSi	Trifluorosilane–d	II–72
F_3N	Nitrogen trifluoride–$^{14}NF_3$	I–16
F_3N	Nitrogen trifluoride–$^{15}NF_3$	II–35
F_3NS	Thionitrosyl trifluoride	II–70
F_3OP	Phosphoryl fluoride	II–76
F_3P	Phosphorus trifluoride	I–19
F_3PS	Thiophosphoryl trifluoride	II–79
F_4Si	Silicon tetrafluoride	I–29
F_5P	Phosphorus pentafluoride	II–114
F_5V	Vanadium pentafluoride	II–117
F_6Ir	Iridium (VI) fluoride	II–121
F_6Mo	Molybdenum (VI) fluoride	I–52
F_6S	Sulfur hexafluoride	I–50
F_6Se	Selenium hexafluoride	I–51
F_6Te	Tellurium hexafluoride	II–120
F_6U	Uranium (VI) fluoride	I–54
F_6W	Tungsten (VI) fluoride	I–53
GeH_3I	Germyl iodide	II–90
GeH_3I	Germyl iodide–d_3	II–91
GeH_4	Germane	I–33
GeH_4	Germane–d_1	I–34
GeH_4	Germane–d_2	I–35
GeH_4	Germane–d_3	I–36
GeH_4	Germane–d_4	I–37
Ge_2H_6	Digermane	II–125
Ge_2H_6	Digermane–d_6	II–126
HNO_3	Nitric acid–$H^{14}NO_3$	II–102
HNO_3	Nitric acid–d–$D^{14}NO_3$	II–103
HNO_3	Nitric acid–$H^{15}NO_3$	II–104
HNO_3	Nitric acid–d–$D^{15}NO_3$	II–105
HN_3	Hydrazoic acid	II–50
HN_3	Hydrazoic acid–d	II–51
H_2O	Water	I–4
H_2O	Water–$H_2{}^{18}O$	II–6
H_2O	Water–d_1	I–5
H_2O	Water–d_2	I–6
H_2O_2	Hydrogen peroxide	II–47
H_2S	Hydrogen sulfide	I–9
H_2S	Hydrogen sulfide-d_2	I–10
H_2S_2	Hydrogen persulfide	II–48
H_2Se	Hydrogen selenide	I–12
H_2Se	Hydrogen selenide-d_1	I–13
H_3N	Ammonia	I–14
H_3N	Ammonia–d_3	I–15
H_3N	Ammonia–t_3	II–34
H_3P	Phosphine	I–17
H_3P	Phosphine–d_3	I–18
H_3Sb	Stibine	I–23
H_3Sb	Stibine–d_3	I–24
H_4Si	Silane	I–25
H_4Si	Silane–d_2	I–26
H_4Si	Silane–d_3	I–27
H_4Si	Silane–d_4	I–28
IF_7	Iodine heptafluoride	II–124
I_3P	Phosphorus triiodide	II–37
I_4H_f	Hafnium tetraiodide	II–67
I_4Si	Silicon tetraiodide	I–32
I_4Ti	Titanium tetraiodide	II–60
I_4Zr	Zirconium tetraiodide	II–63
NO_2	Nitrogen dioxide–$^{14}NO_2$	II–2

Empirical Formula	Name	Volume and Number
NO_2	Nitrogen dioxide–$^{15}NO_2$	II–3
N_2O	Nitrous oxide	I–1
N_2O	Nitrous oxide–$^{14}N^{15}NO$	I–2
N_2O	Nitrous oxide–$^{15}N_2O$	I–3
O_2S	Sulfur dioxide	I–11
O_2S	Sulfur dioxide–$S^{18}O_2$	II–7
O_3	Ozone–$^{16}O_3$	II–4
O_3	Ozone–$^{18}O_3$	II–5
O_3S	Sulfur trioxide	II–33
O_4Os	Osmium tetroxide–$Os^{16}O_4$	II–68
O_4Os	Osmium tetroxide–$Os^{18}O_4$	II–69
O_4Ru	Ruthenium tetroxide	II–64

Compounds Containing Carbon

Empirical Formula	Name	Volume and Number
CBrClO	Carbonyl bromochloride	II–137
CBrClS	Thiocarbonyl bromochloride	II–138
$CBrCl_2F$	Bromodichlorofluoromethane	II–148
$CBrCl_3$	Bromotrichloromethane	I–93
$CBrF_3$	Bromotrifluoromethane	II–141
CBrN	Cyanogen bromide–$^{79}BrCN$	I–66
CBrN	Cyanogen bromide–$^{81}BrCN$	I–67
CBr_2ClF	Dibromochlorofluoromethane	II–149
CBr_2Cl_2	Dibromodichloromethane	I–101
CBr_2F_2	Dibromodifluoromethane	II–147
CBr_2O	Carbonyl bromide	II–131
CBr_3Cl	Tribromochloromethane	I–94
CBr_3F	Tribromofluoromethane	II–145
CBr_4	Carbon tetrabromide	I–78
CClFO	Carbonyl chlorofluoride	II–136
$CClF_3$	Chlorotrifluoromethane	II–140
CClN	Cyanogen chloride–$^{35}ClCN$	I–64
CClN	Cyanogen chloride–$^{37}ClCN$	I–65
CCl_2F_2	Dichlorodifluoromethane	II–146
CCl_2O	Carbonyl chloride	II–130
CCl_2S	Thiocarbonyl chloride	II–133
CCl_3F	Trichlorofluoromethane	II–143
CCl_3I	Trichloroiodomethane	II–144
CCl_4	Carbon tetrachloride	I–77
CFN	Cyanogen fluoride	II–127
CF_2O	Carbonyl fluoride	II–129
CF_2S	Thiocarbonyl fluoride	II–132
CF_3I	Trifluoroiodomethane	II–142
CF_4	Carbon tetrafluoride	I–76
CIN	Cyanogen iodide	II–128
CI_4	Carbon tetraiodide	I–79
COS	Carbonyl sulfide	I–61
CO_2	Carbon dioxide	I–58
CO_2	Carbon dioxide–$^{13}CO_2$	I–59
CS_2	Carbon disulfide	I–60
$CHBr_3$	Tribromomethane	I–91
$CHBr_3$	Tribromomethane–d_1	I–92

Empirical Formula	Name	Volume and Number
$CHCl_3$	Trichloromethane	I–89
$CHCl_3$	Trichloromethane–d_1	I–90
CHF_3	Trifluoromethane	I–88
CHF_3	Trifluoromethane–d	II–139
CHN	Hydrogen cyanide	I–62
CHN	Hydrogen cyanide–d_1	I–63
CHNO	Isocyanic acid	II–134
CHNO	Isocyanic acid–d	II–135
CH_2BrCl	Bromochloromethane	I–102
CH_2BrCl	Bromochloromethane–d_1	I–103
CH_2BrCl	Bromochloromethane–d_2	I–104
CH_2Br_2	Dibromomethane	I–98
CH_2Br_2	Dibromomethane–d_1	I–99
CH_2Br_2	Dibromomethane–d_2	I–100
CH_2Cl_2	Dichloromethane	I–95
CH_2Cl_2	Dichloromethane–d_1	I–96
CH_2Cl_2	Dichloromethane–d_2	I–97
CH_2O	Formaldehyde	I–68
CH_2O	Formaldehyde–d_1	I–69
CH_2O	Formaldehyde–d_2	I–70
CH_2O_2	Formic acid	I–105
CH_2O_2	Formic acid–d_2	I–106
CH_3BO	Borine carbonyl–$^{10}BH_3CO$	II–150
CH_3BO	Borine carbonyl–d_3 $^{10}BD_3CO$	II–151
CH_3BO	Borine carbonyl–$^{11}BH_3CO$	II–152
CH_3BO	Borine carbonyl–d_3 $^{11}BD_3CO$	II–153
CH_3Br	Methylbromide	I–84
CH_3Br	Methylbromide–d_3	I–85
CH_3Cl	Methylchloride	I–82
CH_3Cl	Methylchloride–d_3	I–83
CH_3F	Methylfluoride	I–80
CH_3F	Methylfluoride–d_3	I–81
CH_3GeI_3	Methyltriiodogermane	II–159
CH_3HgI	Methylmercuric iodide	II–154
CH_3I	Methyliodide	I–86
CH_3I	Methyliodide–d_3	I–87
CH_4	Methane	I–71
CH_4	Methane–d_1	I–72
CH_4	Methane–d_2	I–73
CH_4	Methane–d_3	I–74
CH_4	Methane–d_4	I–75
CH_4O	Methanol (Gas)	I–107
CH_4O	Methanol (Liquid)	I–108
CH_4O	Methanol–d_1 (Gas)	I–109
CH_4O	Methanol–d_1 (Liquid)	I–110
CH_4O	Methanol–d_3 (Gas)	I–111
CH_4O	Methanol–d_3 (Liquid)	I–112
CH_4O	Methanol–d_4 (Gas)	I–113
CH_5N	Methylamine	I–114
CH_5N	Methylamine–d_2	I–115
CH_5N	Methylamine–d_3	I–116
CH_5N	Methylamine–d_5	I–117
CH_6Ge	Methylgermane	II–157
CH_6Ge	Methyl–d_3–germane	II–158
CH_6Si	Methylsilane	II–155
CH_6Si	Methylsilane–d_3	II–156

Empirical Formula	Name	Volume and Number
CH_6Sn	Methylstannane	II–160
CH_6Sn	Methylstannane–d_3	II–161
CH_6Sn	Methyl–d_3–stannane	II–162
C_2BrCl	Bromochloroacetylene	II–167
C_2BrI	Bromoiodoacetylene	II–169
C_2Br_2	Dibromoacetylene	II–165
C_2Br_4	Tetrabromoethylene	I–128
C_2Br_6	Hexabromoethane	I–159
C_2ClI	Chloroiodoacetylene	II–168
C_2Cl_2	Dichloroacetylene	II–164
$C_2Cl_2F_2$	trans–1,2–Dichloro–1,2–difluoroethylene	I–138
$C_2Cl_2F_2$	1,1–Dichloro–2,2–difluoroethylene	I–142
C_2Cl_4	Tetrachloroethylene	I–127
C_2Cl_6	Hexachloroethane	I–158
C_2F_3N	Trifluoroacetonitrile	II–170
C_2F_4	Tetrafluoroethylene	I–126
C_2F_6	Hexafluoroethane	I–157
C_2I_2	Diiodoacetylene	II–166
C_2N_2	Cyanogen	II–163
C_2HBr	Bromoacetylene	I–123
C_2HCl	Chloroacetylene	I–122
C_2HF	Fluoroacetylene	I–121
C_2H_2	Acetylene	I–118
C_2H_2	Acetylene–d_1	I–119
C_2H_2	Acetylene–d_2	I–120
$C_2H_2Cl_2$	trans–1,2–Dichloroethylene	I–132
$C_2H_2Cl_2$	trans–1,2–Dichloroethylene–d_1	I–133
$C_2H_2Cl_2$	trans–1,2–Dichloroethylene–d_2	I–134
$C_2H_2Cl_2$	cis–1,2–Dichloroethylene	I–135
$C_2H_2Cl_2$	cis–1,2–Dichloroethylene–d_1	I–136
$C_2H_2Cl_2$	cis–1,2–Dichloroethylene–d_2	I–137
$C_2H_2Cl_2$	1,1–Dichloroethylene	I–139
$C_2H_2Cl_2$	1,1–Dichloroethylene–d_1	I–140
$C_2H_2Cl_2$	1,1–Dichloroethylene–d_2	I–141
$C_2H_2F_2$	cis–1,2–Difluoroethylene	I–129
$C_2H_2F_2$	cis–1,2–Difluoroethylene–d_1	I–130
$C_2H_2F_2$	cis–1,2–Difluoroethylene–d_2	I–131
$C_2H_2F_2$	trans–1,2–Difluoroethylene	II–171
$C_2H_2F_2$	trans–1,2–Difluoroethylene–d_1	II–172
$C_2H_2F_2$	trans–1,2–Difluoroethylene–d_2	II–173
$C_2H_2N_2O$	1,2,5–Oxadiazole	I–147
C_2H_2O	Glyoxal	II–174
C_2H_2O	Glyoxal–d_1	II–175
C_2H_2O	Glyoxal–d_2	II–176
C_2H_3N	Methylcyanide	I–143
C_2H_3N	Methylcyanide–d_3	I–144
C_2H_3N	Methyl isocyanide	I–145
C_2H_3N	Methyl isocyanide–d_3	I–146
C_2H_3OF	Acetyl fluoride	II–177
C_2H_3OF	Acetyl fluoride–d_3	II–178
C_2H_4	Ethylene	I–124
C_2H_4	Ethylene–d_4	I–125
C_2H_4BrCl	1–Bromo–2–chloroethane (trans form)	I–164

Empirical Formula	Name	Volume and Number
C_2H_4BrCl	1–Bromo–2–chloroethane (gauche form)	I–165
$C_2H_4Br_2$	1,2–Dibromoethane (trans form)	I–162
$C_2H_4Br_2$	1,2–Dibromoethane (gauche form)	I–163
$C_2H_4Cl_2$	1,2–Dichloroethane (trans form)	I–160
$C_2H_4Cl_2$	1,2–Dichloroethane (gauche form)	I–161
C_2H_4O	Ethylene oxide	I–149
C_2H_4O	Ethylene oxide–d_4	I–150
C_2H_4O	Acetaldehyde	I–151
C_2H_4O	Acetaldehyde–d_1	I–152
C_2H_4O	Acetaldehyde–d_4	I–153
$C_2H_4O_2$	Methyl formate	I–170
$C_2H_4O_2$	Methyl formate–d_1	I–171
$C_2H_4O_2$	Methyl formate–d_3	I–172
$C_2H_4O_2$	Methyl formate–d_4	I–173
$C_2H_4O_2$	Acetic acid	I–174
$C_2H_4O_2$	Acetic acid–d_1	I–175
C_2H_4Si	Silylacetylene	I–148
C_2H_5Br	Bromoethane	I–168
C_2H_5Cl	Chloroethane	I–167
C_2H_5F	Fluoroethane	I–166
C_2H_5N	Ethylene imine	I–169
C_2H_6	Ethane	I–154
C_2H_6	Ethane–d_3	I–155
C_2H_6	Ethane–d_6	I–156
C_2H_6Cd	Dimethylcadmium	II–181
C_2H_6Cd	Dimethylcadmium–d_6	II–182
C_2H_6Hg	Dimethylmercury	II–183
C_2H_6Hg	Dimethylmercury–d_6	II–184
$C_2H_6N_2$	Azomethane	II–185
$C_2H_6N_2$	Azomethane–d_6	II–186
C_2H_6O	Dimethylether	I–176
C_2H_6O	Dimethylether–d_3	I–177
C_2H_6Zn	Dimethylzinc	II–179
C_2H_6Zn	Dimethylzinc–d_6	II–180
C_3BrF_3	1–Bromo–3,3,3–trifluoropropyne	II–198
C_3BrN	Bromo cyanoacetylene	II–190
C_3ClF_3	1–Chloro–3–3–3–trifluoropropyne	II–197
C_3ClN	Chloro cyanoacetylene	II–189
C_3F_3I	1–Iodo–3–3–3–trifluoropropyne	II–199
C_3IN	Iodo cyanoacetylene	II–191
C_3O_2	Carbon suboxide	II–187
C_3S_2	Carbon subsulfide	II–188
C_3HF_3	Trifluoropropyne	II–195
C_3HF_3	Trifluoropropyne–d	II–196
$C_3H_2N_2$	Malononitrile	I–183
$C_3H_2N_2$	Malononitrile–d_2	I–184
C_3H_3Br	Bromopropadiene	II–193
C_3H_3Br	Propargyl bromide	II–202
C_3H_3Cl	Chloropropadiene	II–192
C_3H_3Cl	Propargyl chloride	II–201
C_3H_3F	Propargyl fluoride	II–200
C_3H_3I	Iodopropadiene	II–194
C_3H_3I	Propargyl iodide	II–203
C_3H_4	Allene	I–178

Empirical Formula	Name	Volume and Number
C_3H_4	Methylacetylene	I–179
C_3H_4	Methylacetylene–d_1	I–180
C_3H_4	Methyl–d_3–acetylene	I–181
C_3H_4	Methylacetylene–d_4	I–182
C_3H_4O	Propenal	I–185
C_3H_5N	Ethylcyanide	I–188
C_3H_6	Cyclopropane	I–186
C_3H_6	Cyclopropane–d_6	I–187
C_3H_6O	Acetone	I–189
C_3H_6O	Acetone–d_3	I–190
C_3H_6O	Acetone–d_6	I–191
$C_3H_6O_2$	Methyl acetate	I–197
$C_3H_6O_2$	Methyl acetate–d_3	I–198
$C_3H_6O_2$	Methyl–d_3–acetate	I–199
$C_3H_6O_2$	Methyl acetate–d_6	I–200
C_3H_8	Propane	I–192
C_3H_8	Propane–d_2	I–193
C_3H_8	Propane–d_3	I–194
C_3H_8	Propane–d_6	I–195
C_3H_8	Propane–d_8	I–196
C_4HBr	Bromodiacetylene	II–205
C_4HCl	Chlorodiacetylene	II–204
C_4HI	Iododiacetylene	II–206
C_4H_2	Butadiyne	I–201
C_4H_4O	Furan	I–202
C_4H_4S	Thiophene	I–203
C_4H_4S	Thiophene–d_4	I–204

Empirical Formula	Name	Volume and Number
C_4H_6	1,3–Butadiene	I–205
C_4H_6	1,3–Butadiene–1–d_1, trans	I–206
C_4H_6	1,3–Butadiene–1,1,2–d_3	I–207
C_4H_6	1,3–Butadiene–1,1,4,4–d_4	I–208
C_4H_6	1,3–Butadiene–d_6	I–209
C_4H_6	2–Butyne	I–210
C_4H_8	Cyclobutane	I–211
C_4H_8	Cyclobutane–d_8	I–212
C_4H_8	2–Methylpropene	I–213
C_4H_8	2–Methyl–d_3–propene–3,3,3–d_3	I–214
C_4H_8O	2–Butanone (trans form)	I–215
$C_4H_8O_2$	1,4–Dioxane	II–207
C_4H_{10}	n–Butane (trans form)	I–216
C_4H_{10}	n–Butane (gauche form)	I–217
C_5H_2O	Diethynyl ketone	II–208
C_6CrO_6	Hexacarbonylchromium	II–210
C_6MoO_6	Hexacarbonylmolybdenum	II–211
C_6N_2	Dicyanodiacetylene	II–209
C_6O_6W	Hexacarbonyltungsten	II–212
C_6H_6	Benzene	I–218
C_6H_6	Benzene–d_6	I–219
C_6H_{12}	Cyclohexane	I–220
C_6H_{12}	Cyclohexane–d_{12}	I–221
$-(CH_2)n-$	Poly–(methylene)$_n$	I–222
$-(CH_2)n-$	Poly–(methylene–d_2)$_n$	I–223